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(54) Title: CRYSTALLINE FGF9 DIMER AND METHODS OF USE

(57) Abstract: The crystal structure of FGF9 has been determined and is shown to exist in a tetragonal space group $I4_1$ with lattice constants a = 151.9 Å and c = 117.2 Å. The crystal may be refined to an R value of R = 22.0 % at 2.6Å resolution. The crystal may be used in drug screening assays. A three-dimensional model of FGF9 is also disclosed, as is a three-dimensional computer image of the three-dimensional structure of FGF9, computer-readable data storage medium encoded with computer-readable data corresponding to the three-dimensional computer image, as well as computers for producing such a three-dimensional representation.

CRYSTALLINE FGF9 DIMER AND METHODS OF USE

FIELD OF THE INVENTION

The present invention relates to certain crystallized fibroblast growth factor 9 (FGF9) dimers. This invention also relates to computational methods for using structure coordinates of the protein complex to screen for and design compounds that interact with FGF9 or homologs thereof and methods of using the crystal structure of FGF9 to design pharmaceuticals.

BACKGROUND OF THE INVENTION

Fibroblast growth factors (FGFs) constitute a family of at least twenty structurally related, heparin binding polypeptides which are expressed in a wide variety of cells and tissues. They stimulate the proliferation of cells from mesenchymal to epithelial and neuroectodermal origin. FGFs share structural similarity, but differ in their target specificity and spatial and temporal expression pattern. The biological response of cells to FGF is mediated through specific, high affinity (Kd 20-500 pM) cell surface receptors that possess intrinsic tyrosine kinase activity and are phosphorylated upon binding of FGF (Coughlin et al 1988). A lower affinity (Kd 2×10^9 M), large capacity (10^6 sites/cell), class of binding sites has also been identified as heparin sulfate moieties of proteoglycans. Heparin sulfates are ubiquitous polysaccharides, composed of repeating disaccharides of variably sulfated, either glucoronate or iduronate and glucosamine residues, arranged in distinct domains which greatly vary in length and sulfation levels. A unique role for these molecules is in the formation of distinct complexes, essential for high affinity binding and

activation of FGF in particular and of other heparin-binding growth factors in general (Yayon et al, 1991; Rapraeger et al 1991).

Ligand and receptor dimerization is a key event in the transmembrane signaling of receptor tyrosine kinases. Receptor dimerization leads to an increase in kinase activity, resulting in autophosphorylation and the induction of diverse biological responses (Schlessinger et al, 1992). Several models have been proposed for the interaction between FGF2-heparin and its receptor (Yayon et al, 1991; Ruoslahti 1991; Spivak-Kroizman et al; 1994, Kan et al; 1993, Guimond 1993; Pantoliano et al, 1994). Previous work utilizing NMR demonstrated that FGF dimers in a symmetric tetramer are formed in the presence of an active heparin decasaccharide (Moy et al, 1997), suggesting that a cis-oriented dimer is the minimal, biologically active structural unit of FGF2. Using defined heparin fragments and soluble FGF receptors further demonstrated that ligand dimerization can significantly enhance binding of FGF2 to FGFR1, dimerization of the receptor and induction of downstream signal transduction pathways. More recently, several studies (Plotnikov et al, 1999; Stauber et al, 2000; Plotnikov et al, 2000) exploring the crystal structure of a complex between FGF2 and FGF1 with the extracellular domains of FGFR1 and FGFR2 have shown a 1:2 molecular ratio of ligands to receptors with no evidence for ligand dimerization, the biological relevance of which has still to be determined.

FGFs share in their primary sequence a homology core of around 120 amino acids, including four cysteine residues, one of which is conserved in all members of the family. The core structure contains 12 antiparallel β strands, organized into a threefold internal symmetry. Equivalent folds have been observed for

the soybean trypsin inhibitor and interleukin IL-1a and b. The best characterized members of the family are FGF1 (aFGF) and FGF2 (bFGF), the structures of which have been determined (Zhang et al, 1991; Zhu et al, 1991). Both are potent mitogens that stimulate proliferation, migration and differentiation of a large variety of cells (Folkman et al, 1987; Rifkin et al, 1989).

FGF9, a recently identified member of the FGF family was originally discovered as a heparin binding glia activating factor (Miyamoto et al, 1993; U.S. patents 5,622,928 and 5,512,460). Human FGF9 codes for a 208 amino acid protein. It shares a 30% overall sequence identity with other FGFs but has a unique spectrum of target cell specificity as it stimulates the proliferation of glia and other fibroblast-like cells but is not mitogenic for endothelial cells (Naruo et al, 1993). The basis for such cell selectivity resides in its differential capacity to bind the different FGF receptors. Recombinant FGF9 binds with high affinity and in a heparin dependent manner to FGFR3, with somewhat less affinity to FGFR2 and with considerably less to FGFR1 (Hecht et al, 1995).

Mutations in FGFR3 have been shown to be responsible for achondroplasia, the most common form of genetic dwarfism. Examination of the sequence of FGFR3 in achondroplasia patients identified a mutation in the transmembrane domain of the receptor.

As reported in WO 96/41523, the entire contents of which are hereby incorporated herein by reference, FGF9 not only specifically binds to the FGFR3, but also specifically activates this receptor without activating the FGFR1 and FGFR4 receptors and, if appropriate concentrations are chosen, without significantly activating

FGFR2. Thus, a pharmaceutical composition comprising a pharmaceutically acceptable carrier and, as an active ingredient, a therapeutically effective amount of FGF9, may be used for stimulating the activity of FGFR3. Similarly, if antagonists of FGF9 could be found, pharmaceutical compositions containing such antagonists could be used to attenuate the activity of FGFR3.

Normal cartilage and bone growth and repair of damage to the cartilage and bone requires a specific and delicate balance between up regulation and down regulation of the activity of the FGFR3. It has been theorized that active FGFR3 is necessary in the initial stages of cartilage-bone differentiation, and, after differentiation, is required for cartilage-bone repair. Thus, a pharmaceutical composition comprising as an active ingredient FGF9, which stimulates the activity of FGFR3, may be used in order to encourage cartilage and bone repair, for example by administration to the site of injury. Furthermore, FGFR3 exists usually temporarily on mesenchymal stem cells and usually disappears after differentiation. Administration of FGF9 may serve to stabilize FGFR3 and thus prolong the period in which it is active prior to differentiation. FGF9 has also a chemotactic affect of FGFR3-carrying cells and can promote migration of such FGFR3 carrying cells, typically mesenchymal stem cells, to a desired site, for example, by injection of FGF9 to the growth plate top of the column.

According to this theory, overactivation of FGFR3 after the stage of initial differentiation of bone and cartilage cells, leads to halted growth, and is probably the cause of achondroplasia. Thus, a pharmaceutical composition comprising as an active ingredient an antagonist of FGF9 which attenuates the activity

of FGFR3, or comprising an FGF9 binding agent (such as an antibody against FGF9), which neutralizes native circulating FGF9, should be used in cases of overactivity of the FGFR3 receptor in differentiated tissues, which causes bone and cartilage growth arrest. Such bone and cartilage growth arrest may lead to achondroplasia dwarfism, or other abnormalities of bone and cartilage growth, for example, multiple hereditary exostosis, solitary hereditary exostosis, hallux valgus deformity, synovial chondromatosis and endochondromas.

The above conditions may be treated with a pharmaceutical composition comprising either an antagonist of FGF9, or an FGF9 binding agent capable of neutralizing native circulating FGF9, which both serve to attenuate the activity of FGFR3.

Thus, FGF9 agonists can be used for the purpose of repair and regeneration of defective articular cartilage, for treatment of achondroplastic patients, for treatment of patients suffering from other growth disturbances and for treatment of physical injuries with poor predicted rate of cartilage and bone growth. They may also be used as interventions for manipulating the rate of growth within growth plates in order to increase the growth rate and/or prevent premature differentiation; or may be used for direct injection into the nucleus pulposus of the fine vertebrae in order to enhance the healing of spine injuries. FGF9 antagonists can be used to suppress the activity of a wild type FGFR3 receptor, for example, in the cases of various types of tumors and the like. See WO 96/41620.

As there is a need for compounds that selectively inhibit FGFR3 or act as a selective agonist for FGFR3, it would be desirable to have improved methods that facilitate the design of such compounds.

The concept of rational drug design involves obtaining the precise three-dimensional molecular structure of a specific protein to permit design of drugs that selectively interact with and adjust the function of that protein. Theoretically, if the structure of a protein having a specified function is known, the function of the protein can be adjusted as desired. This permits a number of diseases and symptoms to be controlled. For example, CAPTOPRIL is a well known drug for controlling hypertension that was developed through rational drug design techniques. CAPTOPRIL inhibits generation of the angiotension-converting enzyme, thereby preventing the constriction of blood vessels. The potential for controlling disease through drugs developed by rational drug design is tremendous. The power of rational drug design has been reviewed by Bugg et al (1993).

A requirement of rational drug design is the production of crystals of the desired target protein which provide for the determination of the detailed atomic structure of both the parent protein and its complex with the pharmaceutical. For this purpose, knowledge of the three-dimensional structure coordinates of FGF9 would be useful. Such information would aid in identifying and designing potential inhibitors and agonists of FGFR3 that in turn are expected to have therapeutic utility.

SUMMARY OF THE INVENTION

The present invention provides crystallized FGF9. The structure coordinates reveal that the crystalline FGF9 shows a symmetric dimer with unique receptor and heparin binding surfaces. FGF9 crystallized in the tetragonal space group $I4_1$ with lattice constants a=151.9 Å, c=117.2 Å. The structure has been refined to an R-value of R=22.0% (R_{free}= 25.2%) at 2.6 Å resolution. The four molecules in the asymmetric unit are arranged in two non-crystallographic dimers with the dimer interface composed partly of residues from N- and C-terminal extensions from the FGF-core structure. Most of the receptor-binding residues identified in FGF1- and FGF2-receptor complexes are buried in the dimer interface with the β8/β9 loop stabilized in a particular conformation by an intramolecular hydrogen bonding network. The potential heparin binding sites are in a pattern distinct from FGF1 and FGF2. The carbohydrate moiety attached at N79 has no structural influences.

The use of the crystal structure to design candidate agonists and antagonists of the FGFR3 may be accomplished in the following fashion. Once the crystal structure of the target (i.e., FGF9) is determined, computer modeling is conducted (using such programs as DOCK (Kuntz et al, 1982) or Multiple Copy Simultaneous Search (MCSS)(Mirankev et al, 1991)) to construct candidate agonist or antagonist compounds based on the crystal structure. These compounds are chemically synthesized and their biological activity is assayed. Preferably, such agonists or antagonists are mutants or fragments of FGF9 itself. For example, a preferred antagonist would be a mutant of FGF9 designed by computer modeling

based on the crystal structure of FGF9, which mutant bonds to the FGFR3 receptor without activating it.

Furthermore, once the three-dimensional structure of a crystal comprising the FGF9 protein is determined, a potential ligand (antagonist or agonist) is examined through the use of computer modeling using a docking program such as GRAM, DOCK, or AUTODOCK (Dunbrack et al, 1997). This procedure can include computer fitting of potential ligands to the FGF9 dimer to ascertain how well the shape and the chemical structure of the potential ligand will complement or interfere with the dimer-dimer interaction (Bugg et al, 1993; West et al 1995)). Computer programs can also be employed to estimate the attraction, repulsion, and stearic hindrance of the ligand to the dimer-dimer binding site. Generally, the tighter the fit (e.g., the lower the stearic hindrance, and/or the greater the attractive force), the more potent the potential drug will be since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug, the more likely that the drug will not interfere with other properties of the FGF9 protein. This will minimize potential side effects due to unwanted interactions with other proteins.

Initially a potential ligand could be obtained by screening a random peptide library produced by recombinant bacteriophage for example, (Scott et al, 1990; Cwirla et al, 1990; Devlin et al, 1990) or a chemical library. A ligand selected in this manner could then be systematically modified by computer modeling programs until one or more promising potential ligands are identified. Such analysis has been shown

to be effective in the development of HIV protease inhibitors (Lam et al, 1994; Wlodawer et al, 1993; Appelt, 1993; Erickson, 1993).

Such computer modeling allows the selection of a finite number of rational chemical modifications, as opposed to the countless number of essentially random chemical modifications that could be made, and of which any one might lead to a useful drug. Each chemical modification requires additional chemical steps, which while being reasonable for the synthesis of a finite number of compounds, quickly becomes overwhelming if all possible modifications needed to be synthesized. Thus, through the use of the three-dimensional structure disclosed herein and computer modeling, a large number of these compounds can be rapidly screened on the computer monitor screen, and a few likely candidates can be determined without the laborious synthesis of untold numbers of compounds.

Once a potential ligand (agonist or antagonist) is identified it can be either selected from a library of chemicals as are commercially available from most large chemical companies including Merck, Glaxo Welcome, Bristol Meyers Squib, Monsanto/Searle, Eli Lilly, Novartis and Pharmacia UpJohn, or alternatively the potential ligand may be synthesized *de novo*. As mentioned above, the *de novo* synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design. The prospective drug can be physically tested to confirm its projected activity. For example, if the activity sought for such a potential ligand is its ability to prevent the binding of FGF9 to its receptor FGFR3, the potential ligand can be placed into any standard binding assay described below to test its effect on the FGF9-FGFR3 interaction. A preferred ligand for the purpose of this assay would be

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one which is capable of binding to FGFR3 with a greater affinity than that of FGF9 for FGFR3. If the assay is conducted with FGFR3 on the surface of living cells, then one can determine whether or not the ligand which binds to FGFR3 causes signaling by the receptor. If it binds but does not cause signaling, then it is an antagonist. If it binds and causes signaling, then it is an agonist.

If the activity sought for such a potential ligand is its ability to bind directly to FGF9, this activity can be detected by means of a standard binding assay whereby the potential ligand may be selected on the basis of its having the capability of binding to FGF9. An antagonist may also be a ligand which binds to FGF9 so as to prevent FGF9 from binding to FGFR3. The ability of the potential antagonist to have this activity may also be detected by means of a simple assay for binding to FGF9 in the presence of FGFR3, as is well known in the art.

Other assays which can be conducted for potential ligands relate to the effect of heparin on FGF9. Potential ligands which interact with the heparin binding pockets of FGF9 may have a significant effect on the activity of FGF9, such as by preventing the heparin-dependent oligomerization thereof. Thus, once a potential ligand which may affect the heparin binding property of FGF9 is selected by means of computer modeling, the ability of the potential ligand to actually interfere with such binding may be determined in a standard binding assay to test its effect on the FGF9-heparin interaction.

When a suitable drug is identified, a supplemental crystal can be grown which comprises a protein-ligand complex formed between the FGF9 protein and the drug. Preferably the crystal effectively diffracts X-rays allowing the determination of

the atomic coordinates of the protein-ligand complex to a resolution of greater than 5.0 Ås, more preferably greater than 3.0 Å, and even more preferably greater than 2.0 Å. The three-dimensional structure of the supplemental crystal can be determined by Molecular Replacement Analysis. Molecular replacement involves using a known three-dimensional structure as a search model to determine the structure of a closely related molecule or protein-ligand complex in a new crystal form. The measured X-ray diffraction properties of the new crystal are compared with the search model structure to compute the position and orientation of the protein in the new crystal. Computer programs that can be used include: X-PLOR and AMORE (Navaza, 1994). Once the position and orientation are known an electron density map can be calculated using the search model to provide X-ray phases. Thereafter, the electron density is inspected for structural differences and the search model is modified to conform to the new structure. Other computer programs that can be used to solve the structures of such crystals include QUANTA, CHARMM, INSIGHT, SYBYL, MACROMODE, and ICM.

For all of the drug screening assays described herein further refinements to the structure of the drug will generally be necessary and can be made by the successive iterations of any and/or all of the steps provided by the particular drug screening assay.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 is a ribbon representation of the FGF9 dimer composed of chains A and D showing the carbohydrate moiety bound to each of the chains.

Figure 3 shows the hydrogen bond network stabilizing the β8/β9 loop. Molecule D is represented with the light colored chain on the left side of the figure, molecule A with darker chain trace on the right side of the figure.

Figure 4 shows a diagram of a system used to carry out the instructions encoded by the storage medium of Figure 4A and 4B.

Figure 5A shows a cross-section of a magnetic storage medium.

Figure 5B shows a cross-section of an optically-readable data storage medium.

DETAILED DESCRIPTION OF PREFERRED EMBODIMENTS

Overall Structure Description

The core unit of the FGF9 structure (Fig. 1) is formed by residues 62 to 193 and is very similar to the structures of FGF1 and FGF2, as expected from the sequence alignment (Plotnikov et al. 1999). Further features of the schematic representation of the FGF9 dimer are expanded upon in the inventors' recent publication (Hecht et al. 2001 Acta Cryst. D57). The rms difference to Ca-atoms of FGF1 (Blaber et al, 1996, and pdb-id 2afg) and FGF2 (Zhang et al, 1991, and pdb-id 2FGF) is 0.8 Å. Major differences (rmsd > 1.5 Å) occur at Thr70/Gly71, where FGF1 and FGF2 have an additional glycine, at the loop Asp88/Ser90, which may be correlated with the C-terminal extension in FGF9, and at Tyr153/Arg161, where in FGF9 an insertion of three (relative to FGF1) or five (relative to FGF2) residues occurs. The loop Glu141/Asn146 shows some variability already in FGF1 and FGF2. Compared to FGF1 the largest difference in Ca-positions in this loop is 3.9 Å (at Ala142) while the largest difference is 1.9 Å (at Ala142) compared to FGF2. The loop

containing in FGF9 the glycosylation site at Asn79 is identical to that of FGF1 and FGF2. N-terminal sequencing and Maldi-mass-spectrometry indicated heterogeneity of the crystallized protein with the major components starting at residues 19, 34, 38, and 42. In the structure, residues become visible in one of the molecules at residue 45 with three flexible residues in an extended conformation turning into a helix between residues 48-62. In the other three molecules of the asymmetric unit the helical part is visible only from residue 52 onward. The C-terminal residues starting from residue 193 form an irregular helix which shows some variability in the four molecules of the asymmetric unit. Together these N– and C-terminal parts form an extension clearly separate from the core structure.

Quaternary Structure

There is increasing evidence for the capacity of FGFs to undergo either spontaneous or heparin induced oligomerization, although the relation of such dimers and higher order oligomers to receptor binding and activation is still unclear. For FGF1 a heparin-linked dimeric structure has been reported (DiGabriele et al, 1998) while for FGF2 in the presence of heparin both monomeric and dimeric structures were observed (Faham et al, 1996). Moreover, chemical cross linking, ultracentrifugation experiments (Herr et al, 1997) and mass spectrometric techniques (Davis et al, 1999) provided evidence of self-oligomerization for FGF2 in the presence and in the absence of heparin. Nevertheless, in the structures of the FGF2 receptor complex (Plotnikov et al, 1999) and the FGF1 receptor complex (Stauber et al, 2000) both FGF molecules are separate and only linked via the receptor molecules. In these structures heparin is postulated to bind into a positively charged groove, created in the

receptor dimer with the two termini bound to the heparin-binding domains of the FGF2 molecules (Plotnikov et al, 1999, Stauber et al, 2000).

FGF9 readily dimerizes under physiological conditions, probably more easily than other FGFs, and dimers of FGF9 are frequently observed by immunoblotting lysates of RCJ3.1C5.18 mesenchymal cells (Garofalo et al, 1999) and L-8. Accordingly, the FGF9 structure, crystallized in the absence of heparin, shows the four molecules of the asymmetric unit organized in two dimers related by non-crystallographic symmetry. The solvent accessible surface area, calculated with Grasp (Nicholls et al, 1991), varies between 8848 $Å^2$ and 9306 $Å^2$ for the individual molecules, depending on the length of the extensions. The surface areas of the dimeric molecules, chains AD and BC, are 15826 $Å^2$ and 15481 $Å^2$, yielding buried surface areas of 2422 $Å^2$ and 2420 $Å^2$ or approximately 1200 $Å^2$ per chain, well above the cutoff value of 400 $Å^2$ per chain used as one of the classification criteria by the Protein Quaternary Structure server PQS (http://pqs.ebi.ac.uk/pqs-doc/pqs-doc.shtml). More than half of this buried surface of the dimer is contributed by the N- and C-terminal extensions, as the buried area per dimer is reduced to 1040 $Å^2$ and 853 $Å^2$ when only the residues 62-193 of the FGF-core structure are used in the calculation. The lack of these structured terminal extensions therefore can be one of the reasons why similar dimer formation has not been observed, in the absence of heparin, in the FGF1 and FGF2 structures. For FGF2 the crystal structure with the highest resolution (pdb-id 1bgf) showed disorder for the N-terminal first 19 to 20 residues (Ago et al, 1991), confirmed by NMR studies of complete FGF2 (Lozano et al, 1998; pdb-id 1rml) which showed disorder for the N-terminal 28 residues (Moy et al 1996). For

FGF1 the crystal structure with the highest resolution (Blaber et al, 1996) showed disorder for the N-terminal 9-10 residues (Blaber et al, 1996; pdb-id 2afg) and for the NMR structure a N-terminally at residue 25 truncated molecule was used (Lozano et al, 1998; pdb-id 1rml).

Dimer Interface

The dimer interface in FGF9 consists mainly of hydrophobic contacts but includes 4 hydrogen bonds and two salt bridges, related by non-crystallographic two-fold symmetry. The hydrogen bonds connect the side chain of Y67 with the side chain of N143 and the side chain of R64 with the backbone carbonyl of V192 where the C-terminal extension starts, while the salt bridges connect R62 with D193, also at the start of the C-terminal extension. The hydrophobic contacts are concentrated in a prominent hydrophobic cluster of the residues L54, L57, I60, L61, P194, V197 and L200 at the base of the structure, close to where the terminal extensions join the core. At the center and top of the core structure P191, L188 together with P189 and the hydrophobic parts of the side chains of R190, W144 and Y145 form an additional, though less pronounced hydrophobic patch. A potentially important structural difference between FGF9 and FGF1 and FGF2 occurs in the dimer interface with the noticeable shift of the β-turn linking β8 and β9 (residues 139-146, corresponding to 96-104 in FGF2). In FGF9, the loop conformation is fixed by a hydrogen bond network involving residues H181, H186, E141 and E142 (Fig. 3). The arrangement is stabilized further by a salt bridge between E142 and R69. Residues from this loop have been implicated in receptor binding (Venkataraman et al, 1999) and in the experimental FGF receptor complexes, where residues from this loop make extensive

contacts to the receptor, the loop has been found to undergo some conformational change upon receptor binding (Plotnikov et al, 1999; Stauber et al, 2000). This conformational adaptation is likely to be much reduced in FGF9 due to the hydrogen bonding network. Stabilization of this loop in a particular conformation by residues not directly involved in receptor binding, as in FGF9, therefore could have significant implications on receptor affinity. In the structure of FGF7 (Ye et al, 1999, pdb-id 1QQK), where E142 and R69 are conserved, the loop is in a conformation similar to FGF1 and FGF2 but lacks the salt bridge. Most likely the loop conformation in FGF9 is influenced by the hydrogen bond between E141 and H181, which is unique to FGF9 and FGF16. Similar interactions could occur in FGF5, which has two glutamines in these places, and in FGF10, which has glutamic acid and lysine.

With the exception of residues from the terminal extensions most of the residues (Fig. 1) involved in the dimer interface in FGF9 correspond to residues identified as belonging to the major receptor binding sites in FGF2 (Venkataraman et al, 1999; Plotnikov et al, 1999; Stauber et al, 2000; Plotnikov et al, 2000). This is particularly true for residues Y67, Y145, L188, I60 and H186, corresponding in FGF2 to Y24, Y103, L140, F17 and L138 and in FGF1 to residues Y15, Y94, L133, Y8 and L131 which were found by Plotnikov et al, 1999, and Stauber et al, 2000, to be in contact with the receptor. These residues are almost completely buried (less than 10 $Å^2$ solvent accessible surface, calculated with Areaimol (CCP4, 1994)) in the FGF9 dimer interface and, in order for them to become accessible to the receptor molecule, dissociation of these pre-formed dimers has to occur at least in FGF9.

In the experimental FGF receptor complexes (Plotnikov et al, 1999; Stauber et al, 2000) both the FGF ligand molecules are separate and linked only by heparin via the receptor molecules. A complete separation of the FGF9 dimer requires the separation of the extensive hydrophobic interactions at the N- and C-terminal extensions. As it seems unlikely that these hydrophobic residues remain exposed to solvent, at least three alternative scenarios can be proposed.

1. At present there is no experimental evidence that residues outside of the core-FGF structure participate in receptor binding although in the FGF1/FGFR2 complex both FGF termini are in the vicinity of the receptor. In addition, preliminary results suggest that a complete deletion of both termini may have no apparent functional implications as evidenced by the capacity of a truncated form to both bind receptor and induce cell proliferation (Adar et al, in preparation). The function of these terminal residues could be therefore to provide stability to the unliganded FGF-molecules, probably correlated with the function as a non-cleaved secretion signal attributed to the 60 N-terminal residues by Revest et al (1999), but become redundant and flexible at receptor binding. It is intriguing to suggest that the observed heparin-independent self association of FGF9 could have physiological significance by rendering the non-receptor bound FGF in a protected, non active form by utilizing the same residues defined for receptor binding for a homotypic dimer interface.

2. These residues remain as a connecting region between the FGF molecules after a conformational change that exposes the buried receptor binding residues. Preliminary modeling suggests that this could be possible with hinge regions

probably in the area of residues 62 and 190-192. In this case the terminal extensions could connect adjacent ligand/receptor complexes to form multimeric assemblies.

3. In the experimental receptor/ligand complexes (Plotnikov et al, 1999, Stauber et al, 2000) the secondary receptor binding sites are different from the sites identified by site directed mutagenesis as influencing receptor binding (Springer et al, 1994, Zhu et al, 1997, Zhu et al, 1998). This discrepancy presently is not clear and may point to the involvement of other determinants in FGF in receptor binding and activation.

At least some of the FGFs, especially FGF3 and FGF16, show in the sequence alignment a similar pattern of hydrophobic and hydrophilic residues in these terminal extensions. However, due to the high sequence diversity and the structural flexibility, still more structural investigations of these homologs is yet required.

Potential Heparin Binding Sites

Heparin binding sites have been structurally identified in the heparin linked FGF1 dimer (DiGabriele et al, 1998; pdb-id 2axm) and in heparin complexes with FGF2 monomers (Faham et al, 1996; pdb-id 1bfb) where prominently interactions of basic residues with the sugars, sulphate or carboxylate groups are involved. The surface of FGF9 contains three clusters of basic residues potentially suitable for heparin binding. At least one of these sites contains a bound sulphate molecule while in the other cases the discrimination between bound water and sulphate is less certain due to the limited resolution. The first site is in a pocket created by the insertion at Tyr153/Arg161 and the sulphate ion is bound to R180, Y163 and the backbone nitrogen of R161. This pocket is at approximately 14 Å

distance from the nearest heparin binding site in FGF1 and FGF2 but could occur also in FGF16, FGF13 and FGF11 which have a highly homologous insertion and identical or homologous residues in position 163 and 180. The second site, where R137, K154 and R161 form a cluster highly suggestive of sulphate binding, is even further away from the FGF1 and FGF2 homologous sites and is located almost on the opposite side of the molecule. A similar arrangement could occur in FGF16 as well, where R161 is replaced by a glutamine. The third site is formed by R173 and R177 which correspond to K118 and R122 in the heparin binding loop in FGF1 (DiGabriele et al, 1998; pdb-id 2axm) and to K125 and K129 in FGF2 (Faham et al, 1996; pdb-id 1bfb). Fitting the heparin structures observed in FGF1 (DiGabriele et al, 1998) and FGF2 (Faham et al, 1996) to FGF9, however, shows that the high affinity heparin binding site described by the residues N28, K126 and Q135 in FGF2 (Faham et al, 1996) is partially blocked in FGF9 by the side chain of F184 which makes the backbone nitrogen atoms less accessible for sulphate binding as observed for FGF2 and FGF1. In the experimental FGF2/FGFR1 complex, this site contains a bound sulphate ion and is proposed to bind the terminal part of heparin (Plotnikov et al, 1999). Sulphate ions visible in the experimental FGF1/FGFR2 complex (Stauber et al, 2000; pdb-id 1DJS), however, seem to correspond well with the potential heparin binding sites on FGF9. In this complex three sulphate ions are bound to FGF1, K128, K118, and R122, probably with contributions by K112 and R119. In FGF9 K183 corresponds to FGF1 K128 and, in addition, R69 is directed very close to the sulphate bound to FGF1 K128. FGF9 R173 and R177 correspond to FGF1 K118 and R122 and only a small adjustment due to F184 would be necessary for similar sulphate binding to the

complex. These fine adjustments in the spatial organization of the heparin binding residues in FGF9 may well coordinate with the distinct structural variants of sulfated domains on heparin sulfates, required for binding and activation of different members of the FGF family as well as of other heparin binding growth factors (Ornitz, 2000).

Computer Representation

The FGF9 X-ray coordinate data, when used in conjunction with a computer programmed with software to translate those coordinates into the 3-dimensional structure of FGF9 may be used for a variety of purposes, especially for purposes relating to drug discovery. Such software for generating 3-dimensional graphical representations are known and commercially available. The ready use of the coordinate data requires that it be stored in a computer-readable format. Thus, in accordance with the present invention, data capable of being displayed as the 3-dimensional structure of FGF9 and portions thereof and their structurally similar homologs is stored in a machine-readable storage medium, which is capable of displaying a graphical 3-dimenslonal representation of the structure.

Therefore, another embodiment of this invention provides a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data which, when used by a machine programmed with instructions for using said data, displays a graphical 3-dimensional representation of a molecule or molecular complex comprising FGF9, or a homolog of said molecule or molecular complex, wherein said homolog comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than about 1.15Å.

Even more preferred is a machine-readable data storage medium that is capable of displaying a graphical 3-dimensional representation of a molecule or molecular complex that is defined by the structure coordinates of all of the amino acids in Figure 2 or a homolog of said molecule or molecular complex, wherein said homolog has a root mean square deviation from the backbone atoms of all of the amino acids in Figure 2 of not more than about 1.15Å.

According to an alternate embodiment, the machine-readable data storage medium comprises a data storage material encoded with a first set of machine-readable data which comprises the Fourier transform of the structure coordinates set forth in Figure 2, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine-readable data comprising the X-ray diffraction pattern of another molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine-readable data.

For example, the Fourier transform of the structure coordinates set forth in Figure 2 may be used to determine at least a portion of the structure coordinates of FGF9.

According to an alternate embodiment, this invention provides a computer for producing a 3-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises all of the FGF9 amino acids, wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said machine-readable data comprises the structure coordinates of FGF9 or portions thereof;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium, for processing said machine-readable data into said 3-dimensional representation; and

(d) an output hardware coupled to said central processing unit, for receiving said 3-dimensional representation.

Figure 4 demonstrates one version of these embodiments. System 10 includes a computer 11 comprising a central processing unit ("CPU") 20, a working memory 22 which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory 24 (such as one or more disk drives or CD-ROM drives), one or more cathode-ray tube ("CRT") display terminals 26, one or more keyboards 28, one or more input lines 30, and one or more output lines 40, all of which are interconnected by a conventional bidirectional system bus 50.

Input hardware 36, coupled to computer 11 by input lines 30, may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems 32 connected by a telephone line or dedicated data line 34. Alternatively or additionally, the input hardware 36 may comprise CD-ROM drives or disk drives 24. In conjunction with display terminal 26, keyboard 28 may also be used as an input device.

Output hardware 46, coupled to computer 11 by output lines 40, may similarly be implemented by conventional devices. By way of example, output hardware 46 may include CRT display terminal 26 for displaying a graphical representation of a binding pocket of this invention using a program such as QUANTA as described herein. Output hardware might also include a printer 42, so that hard copy output may be produced, or a disk drive 24, to store system output for later use.

In operation, CPU 20 coordinates the use of the various input and output devices 36, 46 coordinates data accesses from mass storage 24 and accesses to and from working memory 22, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to components of the hardware system 10 are included as appropriate throughout the following description of the data storage medium.

Figure 5A shows a cross section of a magnetic data storage medium 100 which can be encoded with a machine-readable data that can be carried out by a system such as system 10 of Figure 4. Medium 100 can be a conventional floppy diskette or hard disk, having a suitable substrate 101, which may be conventional, and a suitable coating 102, which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium 100 may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device 24. The magnetic domains of

coating 102 of medium 100 are polarized or oriented so as to encode in manner which may be conventional, machine-readable data such as that described herein, for execution by a system such as system 10 of Figure 4.

Figure 5B shows a cross-section of an optically-readable data storage medium 110 which also can be encoded with such a machine-readable data, or set of instructions, which can be carried out by a system such as system 10 of Figure 4. Medium 110 can be a conventional compact disk read only memory (CD-ROM) or a rewritable medium such as a magneto-optical disk that is optically readable and magneto-optically writable. Medium 100 preferably has a suitable substrate 111, which may be conventional, and a suitable coating 112, which may be conventional, usually of one side of substrate 111.

In the case of CD-ROM, as is well known, coating 112 is reflective and is impressed with a plurality of pits 113 to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating 112. A protective coating 114, which preferably is substantially transparent, is provided on top of coating 112.

In the case of a magneto-optical disk, as is well known, coating 112 has no pits 113, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating 112. The arrangement of the domains encodes the data as described above.

As mentioned above, the FGF9 X-ray coordinate data is useful for screening and identifying drugs that inhibit FGF9. For example, the structure encoded by the data may be computationally evaluated for its ability to associate with putative substrates or ligands. Such compounds that associate with FGF9 may inhibit FGF9, and are potential drug candidates. Additionally or alternatively, the structure encoded by the data may be displayed in a graphical 3-dimensional representation on a computer screen. This allows visual inspection of the structure, as well as visual inspection of the structure's association with the compounds.

Thus according to another embodiment, the method evaluates the potential of a chemical entity to associate with a molecule or molecular complex defined by the structure coordinates of all of the FGF9 amino acids, as set forth in Figure 2, or a homolog of said molecule or molecular complex having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.1Å.

This method comprises the steps of:

a) creating a computer model of the molecular or molecular complex using the structure coordinates as set forth in Figure 2, or a homolog of said molecule or molecular complex having a root mean square deviation from the backbone atoms of said amino acids not more than about 1.15Å;

b) employing computational means to perform a fitting operation between the chemical entity and said computer model of the binding pocket; and

c) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket model.

The term "chemical entity", as used herein, refers to chemical compounds or ligands, complexes of at least two chemical compounds, and fragments of such compounds or complexes.

More preferred is the use of the atomic coordinates of all the amino acids of FGF9 according to Figure 2 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.15Å, to generate a 3-dimensional structure of FGF9.

For the first time, the present invention permits the use of molecular design techniques to identify, select or design potential inhibitors of FGF9, based on the structure of thereof. Such a predictive model is valuable in light of the high costs associated with the preparation and testing of the many diverse compounds that may possibly bind to the FGF9 protein.

According to this invention, a potential FGF9 inhibitor may now be evaluated for its ability to bind a FGF9-like binding pocket prior to its actual synthesis and testing. If a proposed compound is predicted to have insufficient interaction or association with the binding pocket, preparation and testing of the compound is obviated. However, if the computer modeling indicates a strong interaction, the compound may then be obtained and tested for its ability to bind.

A potential inhibitor of a FGF9-like binding pocket may be computationally evaluated by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the FGF9-like binding pockets.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with a FGF9-like binding pocket. This process may begin by visual inspection of, for example, a FGF9-like binding pocket on the computer screen based on the FGF9 structure coordinates in Figure 2 or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within that binding pocket as defined above. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

1. GRID (Goodford, 1985), which is available from Oxford University, Oxford, UK.

2. MCSS (Miranker et al, 1991), which is available from Molecular Simulations, San Diego, CA.

3. AUTODOCK (Goodsell et al, 1990), which is available from Scripps Research Institute, La Jolla, CA.

4. DOCK (Kuntz et al, 1982), which is available from University of California, San Francisco, CA.

Once suitable chemical entities or fragments have been selected, they can be designed or assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the

3-dimensional image displayed on a computer screen in relation to the structure coordinates of FGF9. This would be followed by manual model building using software such as Quanta or Sybyl (Tripos Associates, St. Louis, MO). Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT (Bartlett et al, 1989; Lauri et al, 1994), which is available from the University of California, Berkeley, CA.

2. 3D Database systems, such as ISIS (MDL Information Systems, San Leandro, CA). This area is reviewed in Martin, 1992.

3. HOOK (Eisen et al, 1994), which is available from Molecular Simulations, San Diego, CA.

Instead of proceeding to build an inhibitor of a FGF9-like binding pocket in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other FGF9 binding compounds may be designed as a whole or "*de novo*" using either an empty binding site or optionally including some portion(s) of a known inhibitor(s). There are many *de novo* ligand design methods including:

1. LUDI (Bohm, 1992), which is available from Molecular Simulations Incorporated, San Diego, CA.

2. LEGEND (Nishibata et al, 1991), which is available from Molecular Simulations Incorporated, San Diego, CA.

3. LeapFrog (available from Tripos Associates, St. Louis, MO).

4. SPROUT (Gillet et al, 1993), which is available from the University of Leeds, UK.

Other molecular modeling techniques may also be employed in accordance with this invention (see, e.g., Cohen et al, 1990; Navia et al, 1992; Balbes et al, 1994; Guida, 1994).

Once a compound has been designed or selected by the above methods, the efficiency with which that entity may bind to a FGF9 binding pocket may be tested and optimized by computational evaluation. For example, an effective FGF9 binding pocket inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient FGF9 binding pocket inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, more preferably, not greater than 7 kcal/mole. FGF9 binding pocket inhibitors may interact with the binding pocket in more than one of multiple conformations that are similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

An entity designed or selected as binding to a FGF9 binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 99, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh,

PA, ©1995); AMBER, version 4.1 (P. A. Kollman, University of California at San Francisco, ©1995); QUANTA/CHARMM (Molecular Simulations, Inc., San Diego, CA ©1995); Insight II/Discover (Molecular Simulations, Inc., San Diego, GA ©1995); DelPhi (Molecular Simulations, Inc., San Diego, CA ©1995); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs may be implemented, for instance, using a Silicon Graphics workstation such as an Indigo^2 with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

Another approach enabled by this invention, is the computational screening of small molecule databases for chemical entities or compounds that can bind in whole, or in part, to a FGF9 binding pocket. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarily or by estimated interaction energy (Meng et al, 1992).

According to another embodiment, the invention provides compounds that associate with a FGF9-like binding pocket produced or identified by the method set forth above.

The structure coordinates set forth in Figure 2 can also be used to aid in obtaining structural information about another crystallized molecule or molecular complex. This may be achieved by any of a number of well-known techniques, including molecular replacement.

In order that this invention be more fully understood, the following example is set forth. This example is for the purpose of illustration only and is not to be construed as limiting the scope of the invention in any way.

EXAMPLE:

Materials and Methods

The full-length coding region for human FGF9 (Miyamoto et al, 1993) cDNA was isolated as a BamHI/blunt fragment from pET vector (Kuriyama et al, 1995) and subcloned into the vector pBacPAK9 digested with BglII and SmaI. Plasmids containing the cDNA species in proper orientation were isolated from bacteria, used for transfection into Sf9 cells with purified linearized baculovirus DNA. Screening for recombinant viruses, cloning and propagation or rec. viruses were performed as described (Fiebich et al, 1993). For purification of FGF9 protein from the insect cell serum-free supernatant, it was adjusted to 0.6 M NaCl and purified over a 5 ml HiTrap heparin column (Pharmacia Amersham). FGF9 containing samples were pooled, diluted 1:3 with 20 mM Tris/Cl pH 7.4 and applied to a 5-ml TSK-heparin-affinity FPLC column (TosoHaas). Bound proteins were eluted with a 20ml gradient of 0.4-1.5 M NaCl in buffer A (20 mM Tris/Cl, pH 7.4). Aliquots of 1 ml fraction containing FGF9 were used for SDS/PAGE and for silver staining of the gel.

The protein concentration was measured with a standard assay (BCA, Pierce). For amino-terminal sequencing of glycosylated rh FGF9, 20 mg protein from the biological active fractions (estimated with BALBc-3T3 cells, not shown) were loaded onto a Applied Biosystems 473 A gas-phase protein sequenator. Twenty rounds of Edman degradation were carried out using standard protocols and chemicals supplied by Applied Biosystems (ca. 50% pos. 19 and 50% pos. 34 of the coding region).

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Crystals were grown with the sitting drop method to a typical size of 0.2×0.2×0.2 mm from solutions containing FGF9 at a concentration of 2.1 mg/ml and 2.0 M ammonium sulphate, buffered at pH 5.2 with 0.1 M MES/Tris buffer. The statistics of the native data set, collected at the MPG-GBF beamline BW6 of the DESY synchrotron from a shock-cooled crystal to a resolution of 2.6 Å, are given in Table 1. Indexing and scaling the data set with Mosflm (CCP4, 1994) and Scala (CCP4, 1994) proved the space group to be tetragonal $I4_1$ with lattice constants a=151.9 Å, c=117.2 Å. The asymmetric unit contains four molecules showing clear two-fold symmetry in a pseudo-I4122 arrangement and in addition a pseudo-cubic three-fold axis in the self-rotation function calculated with Glrf (Tong et al, 1997). The structure was solved by molecular replacement. The successful run of EPMR (Kissinger et al, 1999) used the coordinates of FGF1 (Blaber et al, 1996; pdb-id 2afg), modified by replacement of all non-glycine residues by alanine, and identified clearly three of the four molecules in the asymmetric unit with a correlation factor of 0.296. The fourth molecule was placed manually by complementing the third molecule to a dimer identical to the first two molecules. The structure was refined using CNS (Brunger et al, 1998), Refmac (CCP4, 1994), and O (Jones et al, 1991). Water molecules were added using Arpp/Refmac (CCP4, 1994) until the decrease of the free R-factor stopped. In the last stages of the refinement positional restraints for the non-crystallographic symmetry were dropped, but, due to the limited resolution, only grouped temperature factors for main chain and side chain atoms were refined.

TABLE 1
Data Set and Refine Statistics

Space Group	$I4_1$
Unit Cell Parameters	
a (Å)	151.9
c (Å)	117.2
Resolution Range (Å)	39.5-2.6
Unique Reflections	40985
Completeness (%)	99.9 (99.9)
I/sigma(I)	9.5 (3.4)
R_{all} (%)	22.0
R_{free} (%)	25.0
Resolution	40-2.6
nr. residues	624
nr. sugars	10
nr. sulfates	8
nr. waters	141
Coord. Error *	0.18
Core Region (%)‡	90.0
ncs-rms (Å)†	0.58

values in parenthesis are for the highest resolution shell 2.74 Å-2.6 Å

$R_{merge} = (\sum I_i(hkl) - \langle I(hkl)\rangle) / (\sum I_i(hkl)$,
$R_{all} = (\sum F_o(hkl) - F_c(hkl)) / (\sum F_o(hkl)$

* calculated with SIGMAA (CCP4) and ‡ calculated with PROCHECK (CCPR)

† rms deviation of Cα protein atoms related by non-crystallographic symmetry calculated with LSQMAN (Kleywegt et al, 1997)

N-terminal sequencing and Maldi-mass-spectrometry indicated heterogeneity of the crystallized protein with the major components starting at residues

19, 34, 38, and 42 (Swissprot id FGF9_HUMAN). The glycoconjugate is, according to Maldi-mass-spectrometry, of the three-mannosyl insect type with 2 N-acetylglucosamines, 3 mannose and one fucose moiety, a minor component having two fucose molecules, as expected from the expression system. The structure shows clearly in all four molecules at the N79 glycosylation site density for the two N-acetylglucosamines together with one fucose molecule, the rest of the carbohydrate is disordered. In the crystal all four molecules of the asymmetric unit show flexibility of the N-terminal and, to a lesser extent, the C-terminal residues.

The first residue visible in the electron density is in one molecule Leu45 and in the others Thr52, C-terminal residues are visible up to 208, the native C-terminus, in one molecule, to 206 in two others, and to 204 in the last molecule. The average rmsd between all Ca-atoms common to the four molecules in the asymmetric unit is 0.6 and 0.3 for the residues 62 to 193. The final refinement statistics for the model consisting of 623 amino acid residues, 10 carbohydrate, 141 water and 8 sulphate molecules are given in Table 1. The coordinates are set forth in Figure 2.

The foregoing description of the specific embodiments will so fully reveal the general nature of the invention that others can, by applying current knowledge, readily modify and/or adapt for various applications such specific embodiments without undue experimentation and without departing from the generic concept, and, therefore, such adaptations and modifications should and are intended to be comprehended within the meaning and range of equivalents of the disclosed embodiments. It is to be understood that the phraseology or terminology employed herein is for the purpose of description and not of limitation. The means, materials,

and steps for carrying out various disclosed functions may take a variety of alternative forms without departing from the invention. Thus the expressions "means to..." and "means for...", or any method step language, as may be found in the specification above and/or in the claims below, followed by a functional statement, are intended to define and cover whatever structural, physical, chemical or electrical element or structure, or whatever method step, which may now or in the future exist which carries out the recited function, whether or not precisely equivalent to the embodiment or embodiments disclosed in the specification above, i.e., other means or steps for carrying out the same functions can be used; and it is intended that such expressions be given their broadest interpretation.

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WHAT IS CLAIMED IS:

1. An FGF9 crystal in a tetragonal space group $I4_1$ with lattice constants a=151.9 Å and c=117.2 Å.

2. A crystal in accordance with claim 1 refined to an R-value of about 22% at 2.6 Å resolution.

3. A composition consisting essentially of FGF9 in crystalline form.

4. A method of using the crystal of claim 1 in a drug screening assay, comprising:

(a) selecting a potential ligand by performing rational drug design with the three-dimensional structure determined for the crystal, wherein said selecting is performed in conjunction with computer modeling;

(b) contacting the potential ligand with FGF9; and

(c) detecting the binding of the potential ligand for FGF9, wherein a potential drug is selected on the basis of its having the capability of binding to FGF9.

5. A method of using the crystal of claim 1 in a drug screening assay, comprising:

(a) selecting a potential ligand by performing rational drug design with the three-dimensional structure determined for the crystal, wherein said selecting is performed in conjunction with computer modeling;

(b) contacting the potential ligand with FGFR3; and

(c) detecting the binding of the potential ligand to FGFR3, wherein a potential drug is selected on the basis of its having the capability of binding to FGFR3 with a greater affinity than that of FGF9 for FGFR3.

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6. A method of using the crystal of claim 1 in a drug screening assay comprising:

(a) selecting a potential antagonist by performing rational drug design with the three-dimensional structure determined for the crystal, wherein said selecting is performed in conjunction with computer modeling;

(b) adding the potential antagonist to a mixture of FGF9 and FGFR3; and

(c) detecting the ability of the potential antagonist to prevent binding of FGF9 to FGFR3, wherein a potential antagonist that inhibits the binding of FGF9 to FGFR3 is selected as a potential drug.

7. A method in accordance with any one of claims 4-6, wherein said potential ligand or potential antagonist is a mutant or fragment of FGF9.

8. A crystal in accordance with claim 1, wherein the four molecules of the asymmetric unit are organized in two dimers related by non-crystallographic symmetry.

9. A model of FGF9, wherein said model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Figure 2.

10. A computer-assisted method of structure based drug design of bioactive compounds using the model of claim 9, comprising:

providing said model in the form of a computer image generated when the coordinates listed in Figure 2 are analyzed on a computer using a graphical display software program to create an electronic file of said image and visualizing said electronic files on a computer capable of representing said electronic file as a three-dimensional image;

designing a chemical compound using said computer image; and

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chemically synthesizing said chemical compound.

11. A method in accordance with claim 10, wherein said step of designing comprises computational screening of one or more databases of chemical compounds in which the three-dimensional structure of said compounds are known.

12. A three-dimensional computer image of the three-dimensional structure of FGF9.

13. The image of claim 12, wherein said structure substantially conforms with the three-dimensional coordinates listed in Figure 2.

14. A computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said computer-readable data comprises a set of three-dimensional coordinates of FGF9 having a three-dimensional structure that substantially conforms to the atomic coordinates of Figure 2, wherein, using a graphical display software program, said data creates an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

15. A computer for producing a three-dimensional representation of FGF9, wherein said computer comprises:

a computer-readable data storage medium in accordance with claim 14;

a working memory for storing instructions for processing said computer-readable data;

a central-processing unit coupled to said working memory and to said computer-readable data storage medium, for processing said computer-readable data into said three-dimensional representation; and

an output hardware coupled to said central processing unit, for receiving said three-dimensional representation.

FIGURE 1

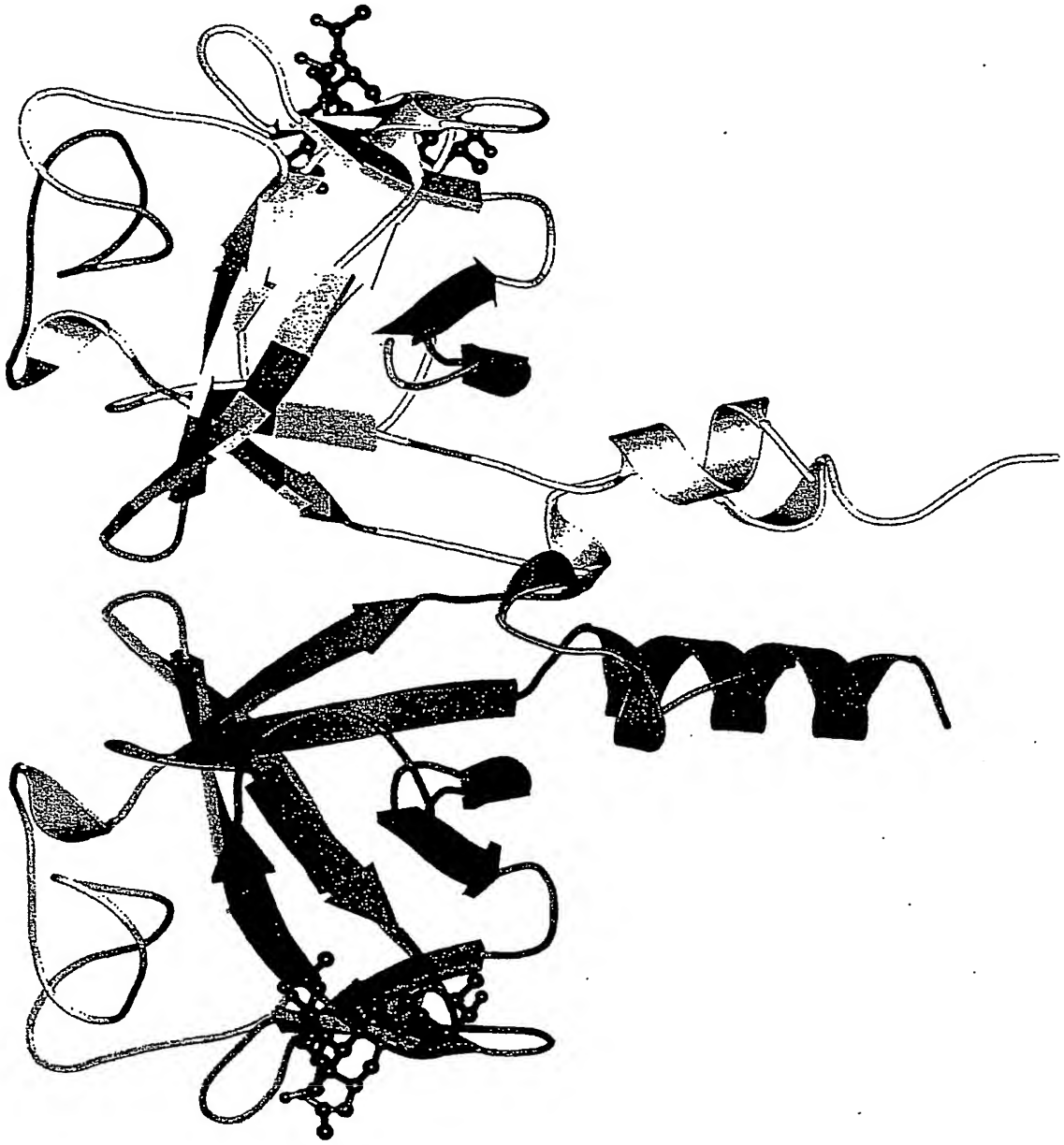


FIGURE 2

REMARK coordinates from minimization and B-factor refinement
REMARK refinement resolution: 500.0 - 2.6 A
REMARK starting r= 0.2186 free_r= 0.2494
REMARK final r= 0.2188 free_r= 0.2500
REMARK rmsd bonds= 0.006201 rmsd angles= 1.30156
REMARK B rmsd for bonded mainchain atoms= $brms_bond_1 target= &bsig_main
REMARK B rmsd for angle mainchain atoms= $brms_angl_1 target= &asig_main
REMARK target= mlf final wa= 1.56562 final rweight=$b_rweight
REMARK md-method= cartesian annealing schedule= slowcool
REMARK starting temperature= 2000 total md steps= 20 * 50
REMARK cycles= 2 coordinate steps= 50 B-factor steps= 30
REMARK sg= I4(1) a= 151.95 b= 151.95 c= 117.23 alpha= 90 beta= 90 gamma= 90
REMARK topology file 1 : CNS_TOPPAR:protein.top
REMARK topology file 2 : CNS_TOPPAR:dna-rna.top
REMARK topology file 3 : CNS_TOPPAR:water.top
REMARK topology file 4 : CNS_TOPPAR:ion.top
REMARK topology file 5 : CNS_TOPPAR:carbohydrate.top
REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNS_TOPPAR:dna-rna_rep.param
REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
REMARK parameter file 4 : CNS_TOPPAR:ion.param
REMARK parameter file 5 : CNS_TOPPAR:carbohydrate.param
REMARK molecular structure file: fgf9_60.mtf
REMARK input coordinates: fgf_r60.xpdb
REMARK reflection file= fgf9h_t-u.refl
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 2.6
REMARK initial B-factor correction applied to fobs :
REMARK B11= 3.191 B22= 3.191 B33= -6.383
REMARK B12= 0.000 B13= 0.000 B23= 0.000
REMARK B-factor correction applied to coordinate array B: 0.876
REMARK bulk solvent: density level= 0.360313 e/A^3, B-factor= 49.9235 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range: 40991 (100.0 %)
REMARK number of unobserved reflections (no entry or |F|=0): 16 (0.0 %)
REMARK number of reflections rejected: 0 (0.0 %)
REMARK total number of reflections used: 40975 (100.0 %)
REMARK number of reflections in working set: 38917 (94.9 %)
REMARK number of reflections in test set: 2058 (5.0 %)
CRYST1 151.950 151.950 117.230 90.00 90.00 90.00 I 41
REMARK FILENAME="/sf/bhf/fgf/cns/fgf9_r60_1.pdb"
REMARK DATE:17-Jul-00 12:21:18 created by user: bhf
REMARK VERSION:1.0

ATOM	1	CB	THR	A	52	62.332	98.192	-4.398	1.00	98.81	A
ATOM	2	OG1	THR	A	52	63.583	98.020	-5.081	1.00	98.81	A
ATOM	3	CG2	THR	A	52	62.575	98.803	-3.021	1.00	98.81	A
ATOM	4	C	THR	A	52	62.621	95.802	-3.722	1.00	100.00	A
ATOM	5	O	THR	A	52	63.042	95.885	-2.565	1.00	100.00	A
ATOM	6	N	THR	A	52	60.404	96.933	-3.410	1.00	100.00	A
ATOM	7	CA	THR	A	52	61.620	96.823	-4.268	1.00	100.00	A
ATOM	8	N	ASP	A	53	62.993	94.840	-4.563	1.00	92.79	A

FIGURE 2 Continued

ATOM	9	CA	ASP	A	53	63.949	93.808	-4.175	1.00	92.79	A
ATOM	10	CB	ASP	A	53	63.826	92.579	-5.082	1.00	100.00	A
ATOM	11	CG	ASP	A	53	62.415	92.033	-5.146	1.00	100.00	A
ATOM	12	OD1	ASP	A	53	61.803	91.824	-4.076	1.00	100.00	A
ATOM	13	OD2	ASP	A	53	61.922	91.804	-6.272	1.00	100.00	A
ATOM	14	C	ASP	A	53	65.371	94.350	-4.275	1.00	92.79	A
ATOM	15	O	ASP	A	53	66.253	93.940	-3.524	1.00	92.79	A
ATOM	16	N	LEU	A	54	65.583	95.272	-5.212	1.00	90.69	A
ATOM	17	CA	LEU	A	54	66.897	95.873	-5.431	1.00	90.69	A
ATOM	18	CB	LEU	A	54	66.838	96.848	-6.613	1.00	88.23	A
ATOM	19	CG	LEU	A	54	68.176	97.443	-7.064	1.00	88.23	A
ATOM	20	CD1	LEU	A	54	68.957	96.396	-7.846	1.00	88.23	A
ATOM	21	CD2	LEU	A	54	67.941	98.675	-7.921	1.00	88.23	A
ATOM	22	C	LEU	A	54	67.411	96.615	-4.194	1.00	90.69	A
ATOM	23	O	LEU	A	54	68.528	96.371	-3.730	1.00	90.69	A
ATOM	24	N	ASP	A	55	66.589	97.521	-3.671	1.00	80.40	A
ATOM	25	CA	ASP	A	55	66.947	98.317	-2.500	1.00	80.40	A
ATOM	26	CB	ASP	A	55	65.906	99.416	-2.276	1.00	100.00	A
ATOM	27	CG	ASP	A	55	65.890	100.436	-3.395	1.00	100.00	A
ATOM	28	OD1	ASP	A	55	65.600	100.054	-4.549	1.00	100.00	A
ATOM	29	OD2	ASP	A	55	66.173	101.620	-3.122	1.00	100.00	A
ATOM	30	C	ASP	A	55	67.095	97.481	-1.235	1.00	80.40	A
ATOM	31	O	ASP	A	55	67.983	97.730	-0.412	1.00	80.40	A
ATOM	32	N	HIS	A	56	66.220	96.495	-1.074	1.00	63.87	A
ATOM	33	CA	HIS	A	56	66.289	95.630	0.092	1.00	63.87	A
ATOM	34	CB	HIS	A	56	65.074	94.707	0.141	1.00	66.67	A
ATOM	35	CG	HIS	A	56	64.965	93.927	1.412	1.00	66.67	A
ATOM	36	CD2	HIS	A	56	64.288	94.181	2.557	1.00	66.67	A
ATOM	37	ND1	HIS	A	56	65.634	92.740	1.618	1.00	66.67	A
ATOM	38	CE1	HIS	A	56	65.374	92.296	2.835	1.00	66.67	A
ATOM	39	NE2	HIS	A	56	64.560	93.152	3.426	1.00	66.67	A
ATOM	40	C	HIS	A	56	67.577	94.811	0.018	1.00	63.87	A
ATOM	41	O	HIS	A	56	68.181	94.489	1.039	1.00	63.87	A
ATOM	42	N	LEU	A	57	67.993	94.491	-1.205	1.00	53.08	A
ATOM	43	CA	LEU	A	57	69.211	93.728	-1.431	1.00	53.08	A
ATOM	44	CB	LEU	A	57	69.279	93.245	-2.881	1.00	67.42	A
ATOM	45	CG	LEU	A	57	70.536	92.450	-3.247	1.00	67.42	A
ATOM	46	CD1	LEU	A	57	70.614	91.187	-2.393	1.00	67.42	A
ATOM	47	CD2	LEU	A	57	70.507	92.099	-4.722	1.00	67.42	A
ATOM	48	C	LEU	A	57	70.414	94.611	-1.128	1.00	53.08	A
ATOM	49	O	LEU	A	57	71.384	94.170	-0.504	1.00	53.08	A
ATOM	50	N	LYS	A	58	70.347	95.859	-1.582	1.00	55.79	A
ATOM	51	CA	LYS	A	58	71.426	96.804	-1.339	1.00	55.79	A
ATOM	52	CB	LYS	A	58	71.071	98.179	-1.911	1.00	90.10	A
ATOM	53	CG	LYS	A	58	71.138	98.270	-3.426	1.00	90.10	A
ATOM	54	CD	LYS	A	58	70.691	99.645	-3.900	1.00	90.10	A
ATOM	55	CE	LYS	A	58	71.106	99.915	-5.342	1.00	90.10	A
ATOM	56	NZ	LYS	A	58	70.597	98.890	-6.292	1.00	90.10	A
ATOM	57	C	LYS	A	58	71.620	96.903	0.170	1.00	55.79	A
ATOM	58	O	LYS	A	58	72.739	97.066	0.659	1.00	55.79	A
ATOM	59	N	GLY	A	59	70.514	96.789	0.900	1.00	49.26	A
ATOM	60	CA	GLY	A	59	70.570	96.861	2.343	1.00	49.26	A
ATOM	61	C	GLY	A	59	71.181	95.611	2.937	1.00	49.26	A
ATOM	62	O	GLY	A	59	71.838	95.680	3.969	1.00	49.26	A
ATOM	63	N	ILE	A	60	70.962	94.462	2.304	1.00	41.77	A
ATOM	64	CA	ILE	A	60	71.521	93.218	2.812	1.00	41.77	A
ATOM	65	CB	ILE	A	60	70.879	91.986	2.124	1.00	45.06	A

FIGURE 2 Continued

ATOM	66	CG2	ILE	A	60	71.789	90.765	2.259	1.00	45.06	A
ATOM	67	CG1	ILE	A	60	69.503	91.720	2.754	1.00	45.06	A
ATOM	68	CD1	ILE	A	60	68.737	90.577	2.134	1.00	45:06	A
ATOM	69	C	ILE	A	60	73.022	93.240	2.597	1.00	41.77	A
ATOM	70	O	ILE	A	60	73.790	92.697	3.401	1.00	41.77	A
ATOM	71	N	LEU	A	61	73.437	93.891	1.515	1.00	41.07	A
ATOM	72	CA	LEU	A	61	74.854	94.022	1.215	1.00	41.07	A
ATOM	73	CB	LEU	A	61	75.054	94.693	-0.141	1.00	57.91	A
ATOM	74	CG	LEU	A	61	74.439	93.933	-1.313	1.00	57.91	A
ATOM	75	CD1	LEU	A	61	74.527	94.770	-2.571	1.00	57.91	A
ATOM	76	CD2	LEU	A	61	75.151	92.605	-1.482	1.00	57.91	A
ATOM	77	C	LEU	A	61	75.497	94.870	2.309	1.00	41.07	A
ATOM	78	O	LEU	A	61	76.710	94.810	2.516	1.00	41.07	A
ATOM	79	N	ARG	A	62	74.676	95.645	3.015	1.00	36.78	A
ATOM	80	CA	ARG	A	62	75.170	96.502	4.089	1.00	36.78	A
ATOM	81	CB	ARG	A	62	74.511	97.891	4.021	1.00	66.13	A
ATOM	82	CG	ARG	A	62	74.561	98.600	2.662	1.00	66.13	A
ATOM	83	CD	ARG	A	62	75.980	98.774	2.147	1.00	66.13	A
ATOM	84	NE	ARG	A	62	76.094	99.682	0.996	1.00	66.13	A
ATOM	85	CZ	ARG	A	62	75.475	99.532	-0.177	1.00	66.13	A
ATOM	86	NH1	ARG	A	62	74.663	98.505	-0.398	1.00	66.13	A
ATOM	87	NH2	ARG	A	62	75.693	100.407	-1.146	1.00	66.13	A
ATOM	88	C	ARG	A	62	74.951	95.912	5.490	1.00	36.78	A
ATOM	89	O	ARG	A	62	75.022	96.637	6.479	1.00	36.78	A
ATOM	90	N	ARG	A	63	74.680	94.610	5.582	1.00	40.59	A
ATOM	91	CA	ARG	A	63	74.467	93.975	6.889	1.00	40.59	A
ATOM	92	CB	ARG	A	63	73.892	92.558	6.732	1.00	57.49	A
ATOM	93	CG	ARG	A	63	72.488	92.476	6.154	1.00	57.49	A
ATOM	94	CD	ARG	A	63	71.481	93.211	7.009	1.00	57.49	A
ATOM	95	NE	ARG	A	63	70.148	93.208	6.412	1.00	57.49	A
ATOM	96	CZ	ARG	A	63	69.265	92.222	6.545	1.00	57.49	A
ATOM	97	NH1	ARG	A	63	69.563	91.142	7.260	1.00	57.49	A
ATOM	98	NH2	ARG	A	63	68.075	92.322	5.968	1.00	57.49	A
ATOM	99	C	ARG	A	63	75.777	93.891	7.680	1.00	40.59	A
ATOM	100	O	ARG	A	63	76.828	93.549	7.128	1.00	40.59	A
ATOM	101	N	ARG	A	64	75.706	94.184	8.976	1.00	38.46	A
ATOM	102	CA	ARG	A	64	76.886	94.149	9.825	1.00	38.46	A
ATOM	103	CB	ARG	A	64	77.596	95.506	9.787	1.00	37.19	A
ATOM	104	CG	ARG	A	64	77.879	96.081	8.411	1.00	37.19	A
ATOM	105	CD	ARG	A	64	79.195	95.593	7.846	1.00	37.19	A
ATOM	106	NE	ARG	A	64	79.497	96.230	6.567	1.00	37.19	A
ATOM	107	CZ	ARG	A	64	78.937	95.896	5.405	1.00	37.19	A
ATOM	108	NH1	ARG	A	64	78.039	94.918	5.351	1.00	37.19	A
ATOM	109	NH2	ARG	A	64	79.272	96.546	4.291	1.00	37.19	A
ATOM	110	C	ARG	A	64	76.551	93.851	11.284	1.00	38.46	A
ATOM	111	O	ARG	A	64	75.391	93.802	11.689	1.00	38.46	A
ATOM	112	N	GLN	A	65	77.603	93.645	12.063	1.00	37.51	A
ATOM	113	CA	GLN	A	65	77.509	93.439	13.497	1.00	37.51	A
ATOM	114	CB	GLN	A	65	77.958	92.040	13.900	1.00	38.80	A
ATOM	115	CG	GLN	A	65	77.133	90.900	13.350	1.00	38.80	A
ATOM	116	CD	GLN	A	65	77.536	89.564	13.965	1.00	38.80	A
ATOM	117	OE1	GLN	A	65	77.282	89.313	15.148	1.00	38.80	A
ATOM	118	NE2	GLN	A	65	78.180	88.709	13.168	1.00	38.80	A
ATOM	119	C	GLN	A	65	78.546	94.453	13.989	1.00	37.51	A
ATOM	120	O	GLN	A	65	79.556	94.680	13.313	1.00	37.51	A
ATOM	121	N	LEU	A	66	78.286	95.087	15.129	1.00	35.76	A
ATOM	122	CA	LEU	A	66	79.223	96.060	15.690	1.00	35.76	A

FIGURE 2 Continued

ATOM	123	CB	LEU	A	66	78.543	97.380	16.042	1.00	36.00	A
ATOM	124	CG	LEU	A	66	78.720	98.549	15.082	1.00	36.00	A
ATOM	125	CD1	LEU	A	66	78.392	99.829	15.846	1.00	36.00	A
ATOM	126	CD2	LEU	A	66	80.139	98.613	14.542	1.00	36.00	A
ATOM	127	C	LEU	A	66	79.844	95.496	16.941	1.00	35.76	A
ATOM	128	O	LEU	A	66	79.228	95.474	18.009	1.00	35.76	A
ATOM	129	N	TYR	A	67	81.077	95.044	16.795	1.00	35.94	A
ATOM	130	CA	TYR	A	67	81.812	94.458	17.894	1.00	35.94	A
ATOM	131	CB	TYR	A	67	82.755	93.388	17.348	1.00	35.96	A
ATOM	132	CG	TYR	A	67	83.622	92.763	18.401	1.00	35.96	A
ATOM	133	CD1	TYR	A	67	83.070	91.942	19.386	1.00	35.96	A
ATOM	134	CE1	TYR	A	67	83.857	91.388	20.371	1.00	35.96	A
ATOM	135	CD2	TYR	A	67	84.995	93.015	18.433	1.00	35.96	A
ATOM	136	CE2	TYR	A	67	85.798	92.466	19.420	1.00	35.96	A
ATOM	137	CZ	TYR	A	67	85.222	91.649	20.386	1.00	35.96	A
ATOM	138	OH	TYR	A	67	86.014	91.068	21.350	1.00	35.96	A
ATOM	139	C	TYR	A	67	82.602	95.527	18.645	1.00	35.94	A
ATOM	140	O	TYR	A	67	83.447	96.220	18.073	1.00	35.94	A
ATOM	141	N	CYS	A	68	82.319	95.671	19.931	1.00	36.87	A
ATOM	142	CA	CYS	A	68	83.032	96.650	20.731	1.00	36.87	A
ATOM	143	CB	CYS	A	68	82.143	97.185	21.859	1.00	39.17	A
ATOM	144	SG	CYS	A	68	82.931	98.454	22.876	1.00	39.17	A
ATOM	145	C	CYS	A	68	84.277	96.012	21.325	1.00	36.87	A
ATOM	146	O	CYS	A	68	84.257	94.847	21.726	1.00	36.87	A
ATOM	147	N	ARG	A	69	85.354	96.791	21.376	1.00	38.81	A
ATOM	148	CA	ARG	A	69	86.632	96.343	21.918	1.00	38.81	A
ATOM	149	CB	ARG	A	69	87.575	97.541	22.062	1.00	84.60	A
ATOM	150	CG	ARG	A	69	89.025	97.200	22.369	1.00	84.60	A
ATOM	151	CD	ARG	A	69	89.867	97.018	21.112	1.00	84.60	A
ATOM	152	NE	ARG	A	69	90.140	95.610	20.826	1.00	84.60	A
ATOM	153	CZ	ARG	A	69	90.956	95.178	19.866	1.00	84.60	A
ATOM	154	NH1	ARG	A	69	91.591	96.043	19.083	1.00	84.60	A
ATOM	155	NH2	ARG	A	69	91.143	93.874	19.691	1.00	84.60	A
ATOM	156	C	ARG	A	69	86.463	95.638	23.270	1.00	38.81	A
ATOM	157	O	ARG	A	69	87.255	94.764	23.617	1.00	38.81	A
ATOM	158	N	THR	A	70	85.434	95.999	24.032	1.00	39.56	A
ATOM	159	CA	THR	A	70	85.217	95.367	25.333	1.00	39.56	A
ATOM	160	CB	THR	A	70	84.213	96.149	26.197	1.00	38.85	A
ATOM	161	OG1	THR	A	70	82.985	96.325	25.472	1.00	38.85	A
ATOM	162	CG2	THR	A	70	84.806	97.499	26.604	1.00	38.85	A
ATOM	163	C	THR	A	70	84.718	93.937	25.236	1.00	39.56	A
ATOM	164	O	THR	A	70	84.504	93.286	26.254	1.00	39.56	A
ATOM	165	N	GLY	A	71	84.519	93.455	24.014	1.00	39.63	A
ATOM	166	CA	GLY	A	71	84.059	92.092	23.828	1.00	39.63	A
ATOM	167	C	GLY	A	71	82.583	91.904	23.522	1.00	39.63	A
ATOM	168	O	GLY	A	71	82.109	90.770	23.480	1.00	39.63	A
ATOM	169	N	PHE	A	72	81.854	92.988	23.277	1.00	35.62	A
ATOM	170	CA	PHE	A	72	80.430	92.854	23.009	1.00	35.62	A
ATOM	171	CB	PHE	A	72	79.618	93.513	24.131	1.00	36.28	A
ATOM	172	CG	PHE	A	72	79.950	93.009	25.507	1.00	36.28	A
ATOM	173	CD1	PHE	A	72	81.047	93.519	26.207	1.00	36.28	A
ATOM	174	CD2	PHE	A	72	79.171	92.018	26.105	1.00	36.28	A
ATOM	175	CE1	PHE	A	72	81.362	93.050	27.494	1.00	36.28	A
ATOM	176	CE2	PHE	A	72	79.471	91.537	27.390	1.00	36.28	A
ATOM	177	CZ	PHE	A	72	80.570	92.052	28.087	1.00	36.28	A
ATOM	178	C	PHE	A	72	79.928	93.398	21.682	1.00	35.62	A
ATOM	179	O	PHE	A	72	80.457	94.363	21.144	1.00	35.62	A

FIGURE 2 Continued

ATOM	180	N	HIS	A	73	78.886	92.764	21.158	1.00	33.67	A
ATOM	181	CA	HIS	A	73	78.274	93.213	19.918	1.00	33.67	A
ATOM	182	CB	HIS	A	73	77.775	92.037	19.073	1.00	40.05	A
ATOM	183	CG	HIS	A	73	78.866	91.242	18.432	1.00	40.05	A
ATOM	184	CD2	HIS	A	73	79.525	91.415	17.261	1.00	40.05	A
ATOM	185	ND1	HIS	A	73	79.401	90.110	19.008	1.00	40.05	A
ATOM	186	CE1	HIS	A	73	80.340	89.618	18.220	1.00	40.05	A
ATOM	187	NE2	HIS	A	73	80.436	90.390	17.152	1.00	40.05	A
ATOM	188	C	HIS	A	73	77.093	94.061	20.338	1.00	33.67	A
ATOM	189	O	HIS	A	73	76.386	93.724	21.293	1.00	33.67	A
ATOM	190	N	LEU	A	74	76.877	95.157	19.621	1.00	33.41	A
ATOM	191	CA	LEU	A	74	75.773	96.057	19.923	1.00	33.41	A
ATOM	192	CB	LEU	A	74	75.961	97.379	19.172	1.00	43.56	A
ATOM	193	CG	LEU	A	74	75.037	98.526	19.589	1.00	43.56	A
ATOM	194	CD1	LEU	A	74	75.582	99.142	20.841	1.00	43.56	A
ATOM	195	CD2	LEU	A	74	74.971	99.582	18.510	1.00	43.56	A
ATOM	196	C	LEU	A	74	74.411	95.454	19.552	1.00	33.41	A
ATOM	197	O	LEU	A	74	74.210	94.973	18.436	1.00	33.41	A
ATOM	198	N	GLU	A	75	73.476	95.496	20.493	1.00	35.72	A
ATOM	199	CA	GLU	A	75	72.131	94.981	20.268	1.00	35.72	A
ATOM	200	CB	GLU	A	75	71.783	93.910	21.302	1.00	45.77	A
ATOM	201	CG	GLU	A	75	72.607	92.658	21.221	1.00	45.77	A
ATOM	202	CD	GLU	A	75	72.372	91.752	22.403	1.00	45.77	A
ATOM	203	OE1	GLU	A	75	72.686	92.158	23.541	1.00	45.77	A
ATOM	204	OE2	GLU	A	75	71.868	90.630	22.199	1.00	45.77	A
ATOM	205	C	GLU	A	75	71.098	96.094	20.375	1.00	35.72	A
ATOM	206	O	GLU	A	75	71.121	96.895	21.312	1.00	35.72	A
ATOM	207	N	ILE	A	76	70.188	96.137	19.411	1.00	35.50	A
ATOM	208	CA	ILE	A	76	69.114	97.119	19.409	1.00	35.50	A
ATOM	209	CB	ILE	A	76	69.074	97.892	18.087	1.00	29.67	A
ATOM	210	CG2	ILE	A	76	67.936	98.899	18.119	1.00	29.67	A
ATOM	211	CG1	ILE	A	76	70.415	98.584	17.844	1.00	29.67	A
ATOM	212	CD1	ILE	A	76	70.513	99.261	16.489	1.00	29.67	A
ATOM	213	C	ILE	A	76	67.815	96.320	19.576	1.00	35.50	A
ATOM	214	O	ILE	A	76	67.299	95.727	18.619	1.00	35.50	A
ATOM	215	N	PHE	A	77	67.297	96.298	20.800	1.00	38.63	A
ATOM	216	CA	PHE	A	77	66.081	95.552	21.109	1.00	38.63	A
ATOM	217	CB	PHE	A	77	66.041	95.241	22.604	1.00	45.88	A
ATOM	218	CG	PHE	A	77	67.023	94.195	23.022	1.00	45.88	A
ATOM	219	CD1	PHE	A	77	66.796	92.855	22.734	1.00	45.88	A
ATOM	220	CD2	PHE	A	77	68.198	94.547	23.671	1.00	45.88	A
ATOM	221	CE1	PHE	A	77	67.736	91.878	23.089	1.00	45.88	A
ATOM	222	CE2	PHE	A	77	69.135	93.576	24.025	1.00	45.88	A
ATOM	223	CZ	PHE	A	77	68.900	92.240	23.730	1.00	45.88	A
ATOM	224	C	PHE	A	77	64.778	96.222	20.690	1.00	38.63	A
ATOM	225	O	PHE	A	77	64.693	97.451	20.575	1.00	38.63	A
ATOM	226	N	PRO	A	78	63.734	95.411	20.463	1.00	51.93	A
ATOM	227	CD	PRO	A	78	63.715	93.942	20.576	1.00	44.46	A
ATOM	228	CA	PRO	A	78	62.421	95.926	20.055	1.00	51.93	A
ATOM	229	CB	PRO	A	78	61.557	94.669	19.992	1.00	44.46	A
ATOM	230	CG	PRO	A	78	62.561	93.576	19.683	1.00	44.46	A
ATOM	231	C	PRO	A	78	61.873	96.958	21.040	1.00	51.93	A
ATOM	232	O	PRO	A	78	61.151	97.869	20.640	1.00	51.93	A
ATOM	233	N	ASN	A	79	62.210	96.822	22.324	1.00	45.34	A
ATOM	234	CA	ASN	A	79	61.725	97.791	23.298	1.00	45.34	A
ATOM	235	CB	ASN	A	79	61.605	97.187	24.702	1.00	48.61	A
ATOM	236	CG	ASN	A	79	62.896	96.597	25.218	1.00	48.61	A

FIGURE 2 Continued

ATOM	237	OD1	ASN	A	79	63.992	97.057	24.900	1.00	48.61	A
ATOM	238	ND2	ASN	A	79	62.732	95.578	26.057	1.00	48.61	A
ATOM	239	C	ASN	A	79	62.519	99.092	23.373	1.00	45.34	A
ATOM	240	O	ASN	A	79	62.285	99.905	24.265	1.00	45.34	A
ATOM	241	N	GLY	A	80	63.448	99.296	22.440	1.00	37.82	A
ATOM	242	CA	GLY	A	80	64.205	100.539	22.422	1.00	37.82	A
ATOM	243	C	GLY	A	80	65.462	100.531	23.261	1.00	37.82	A
ATOM	244	O	GLY	A	80	66.243	101.484	23.249	1.00	37.82	A
ATOM	245	N	THR	A	81	65.648	99.445	23.996	1.00	41.20	A
ATOM	246	CA	THR	A	81	66.808	99.263	24.851	1.00	41.20	A
ATOM	247	CB	THR	A	81	66.494	98.178	25.909	1.00	52.59	A
ATOM	248	OG1	THR	A	81	65.862	98.805	27.035	1.00	52.59	A
ATOM	249	CG2	THR	A	81	67.747	97.431	26.351	1.00	52.59	A
ATOM	250	C	THR	A	81	68.045	98.892	24.026	1.00	41.20	A
ATOM	251	O	THR	A	81	67.939	98.285	22.954	1.00	41.20	A
ATOM	252	N	ILE	A	82	69.214	99.292	24.515	1.00	48.38	A
ATOM	253	CA	ILE	A	82	70.471	99.000	23.843	1.00	48.38	A
ATOM	254	CB	ILE	A	82	71.226	100.285	23.488	1.00	35.38	A
ATOM	255	CG2	ILE	A	82	72.571	99.939	22.852	1.00	35.38	A
ATOM	256	CG1	ILE	A	82	70.371	101.154	22.565	1.00	35.38	A
ATOM	257	CD1	ILE	A	82	70.012	100.498	21.256	1.00	35.38	A
ATOM	258	C	ILE	A	82	71.307	98.189	24.819	1.00	48.38	A
ATOM	259	O	ILE	A	82	71.405	98.530	26.001	1.00	48.38	A
ATOM	260	N	GLN	A	83	71.917	97.118	24.329	1.00	52.04	A
ATOM	261	CA	GLN	A	83	72.709	96.252	25.190	1.00	52.04	A
ATOM	262	CB	GLN	A	83	71.803	95.161	25.761	1.00	80.70	A
ATOM	263	CG	GLN	A	83	72.254	94.568	27.073	1.00	80.70	A
ATOM	264	CD	GLN	A	83	71.400	93.376	27.485	1.00	80.70	A
ATOM	265	OE1	GLN	A	83	70.179	93.369	27.296	1.00	80.70	A
ATOM	266	NE2	GLN	A	83	72.040	92.366	28.064	1.00	80.70	A
ATOM	267	C	GLN	A	83	73.833	95.616	24.383	1.00	52.04	A
ATOM	268	O	GLN	A	83	73.867	95.728	23.156	1.00	52.04	A
ATOM	269	N	GLY	A	84	74.750	94.949	25.073	1.00	38.67	A
ATOM	270	CA	GLY	A	84	75.844	94.302	24.385	1.00	38.67	A
ATOM	271	C	GLY	A	84	75.796	92.805	24.623	1.00	38.67	A
ATOM	272	O	GLY	A	84	75.304	92.364	25.664	1.00	38.67	A
ATOM	273	N	THR	A	85	76.290	92.025	23.659	1.00	40.58	A
ATOM	274	CA	THR	A	85	76.321	90.568	23.786	1.00	40.58	A
ATOM	275	CB	THR	A	85	75.135	89.868	23.079	1.00	33.27	A
ATOM	276	OG1	THR	A	85	75.306	88.451	23.194	1.00	33.27	A
ATOM	277	CG2	THR	A	85	75.099	90.207	21.600	1.00	33.27	A
ATOM	278	C	THR	A	85	77.587	89.978	23.190	1.00	40.58	A
ATOM	279	O	THR	A	85	78.081	90.432	22.151	1.00	40.58	A
ATOM	280	N	ARG	A	86	78.099	88.951	23.855	1.00	40.42	A
ATOM	281	CA	ARG	A	86	79.298	88.273	23.397	1.00	40.42	A
ATOM	282	CB	ARG	A	86	79.932	87.503	24.556	1.00	70.68	A
ATOM	283	CG	ARG	A	86	80.523	88.407	25.615	1.00	70.68	A
ATOM	284	CD	ARG	A	86	81.144	87.617	26.756	1.00	70.68	A
ATOM	285	NE	ARG	A	86	81.950	88.468	27.632	1.00	70.68	A
ATOM	286	CZ	ARG	A	86	83.042	89.129	27.244	1.00	70.68	A
ATOM	287	NH1	ARG	A	86	83.467	89.039	25.987	1.00	70.68	A
ATOM	288	NH2	ARG	A	86	83.715	89.880	28.111	1.00	70.68	A
ATOM	289	C	ARG	A	86	78.985	87.327	22.232	1.00	40.42	A
ATOM	290	O	ARG	A	86	79.860	87.004	21.436	1.00	40.42	A
ATOM	291	N	LYS	A	87	77.726	86.915	22.118	1.00	42.09	A
ATOM	292	CA	LYS	A	87	77.316	85.990	21.065	1.00	42.09	A
ATOM	293	CB	LYS	A	87	75.871	85.541	21.301	1.00	79.48	A

FIGURE 2 Continued

ATOM	294	CG	LYS	A	87	75.595	85.082	22.728	1.00	79.48	A
ATOM	295	CD	LYS	A	87	76.401	83.843	23.133	1.00	79.48	A
ATOM	296	CE	LYS	A	87	75.866	82.573	22.474	1.00	79.48	A
ATOM	297	NZ	LYS	A	87	76.588	81.349	22.918	1.00	79.48	A
ATOM	298	C	LYS	A	87	77.456	86.563	19.651	1.00	42.09	A
ATOM	299	O	LYS	A	87	77.157	87.733	19.402	1.00	42.09	A
ATOM	300	N	ASP	A	88	77.924	85.727	18.728	1.00	33.81	A
ATOM	301	CA	ASP	A	88	78.084	86.131	17.339	1.00	33.81	A
ATOM	302	CB	ASP	A	88	79.134	85.251	16.652	1.00	40.10	A
ATOM	303	CG	ASP	A	88	79.427	85.688	15.228	1.00	40.10	A
ATOM	304	OD1	ASP	A	88	79.168	86.859	14.884	1.00	40.10	A
ATOM	305	OD2	ASP	A	88	79.934	84.864	14.446	1.00	40.10	A
ATOM	306	C	ASP	A	88	76.726	85.965	16.678	1.00	33.81	A
ATOM	307	O	ASP	A	88	75.917	85.154	17.121	1.00	33.81	A
ATOM	308	N	HIS	A	89	76.465	86.750	15.641	1.00	37.93	A
ATOM	309	CA	HIS	A	89	75.197	86.678	14.924	1.00	37.93	A
ATOM	310	CB	HIS	A	89	75.188	85.472	13.974	1.00	49.61	A
ATOM	311	CG	HIS	A	89	76.040	85.648	12.753	1.00	49.61	A
ATOM	312	CD2	HIS	A	89	75.749	86.154	11.528	1.00	49.61	A
ATOM	313	ND1	HIS	A	89	77.366	85.271	12.704	1.00	49.61	A
ATOM	314	CE1	HIS	A	89	77.852	85.534	11.502	1.00	49.61	A
ATOM	315	NE2	HIS	A	89	76.891	86.070	10.769	1.00	49.61	A
ATOM	316	C	HIS	A	89	73.949	86.625	15.821	1.00	37.93	A
ATOM	317	O	HIS	A	89	72.981	85.930	15.505	1.00	37.93	A
ATOM	318	N	SER	A	90	73.962	87.357	16.932	1.00	38.43	A
ATOM	319	CA	SER	A	90	72.804	87.383	17.821	1.00	38.43	A
ATOM	320	CB	SER	A	90	73.128	88.155	19.100	1.00	59.03	A
ATOM	321	OG	SER	A	90	73.433	89.506	18.806	1.00	59.03	A
ATOM	322	C	SER	A	90	71.635	88.054	17.083	1.00	38.43	A
ATOM	323	O	SER	A	90	71.833	88.940	16.255	1.00	38.43	A
ATOM	324	N	ARG	A	91	70.421	87.625	17.400	1.00	39.55	A
ATOM	325	CA	ARG	A	91	69.217	88.135	16.760	1.00	39.55	A
ATOM	326	CB	ARG	A	91	67.986	87.582	17.487	1.00	62.11	A
ATOM	327	CG	ARG	A	91	66.648	88.005	16.898	1.00	62.11	A
ATOM	328	CD	ARG	A	91	65.487	87.392	17.666	1.00	62.11	A
ATOM	329	NE	ARG	A	91	64.208	87.973	17.262	1.00	62.11	A
ATOM	330	CZ	ARG	A	91	63.080	87.875	17.964	1.00	62.11	A
ATOM	331	NH1	ARG	A	91	63.062	87.210	19.114	1.00	62.11	A
ATOM	332	NH2	ARG	A	91	61.973	88.465	17.528	1.00	62.11	A
ATOM	333	C	ARG	A	91	69.127	89.652	16.694	1.00	39.55	A
ATOM	334	O	ARG	A	91	68.736	90.227	15.673	1.00	39.55	A
ATOM	335	N	PHE	A	92	69.486	90.311	17.785	1.00	37.77	A
ATOM	336	CA	PHE	A	92	69.380	91.753	17.817	1.00	37.77	A
ATOM	337	CB	PHE	A	92	68.732	92.149	19.133	1.00	39.75	A
ATOM	338	CG	PHE	A	92	67.344	91.613	19.276	1.00	39.75	A
ATOM	339	CD1	PHE	A	92	66.322	92.078	18.441	1.00	39.75	A
ATOM	340	CD2	PHE	A	92	67.056	90.611	20.204	1.00	39.75	A
ATOM	341	CE1	PHE	A	92	65.033	91.551	18.527	1.00	39.75	A
ATOM	342	CE2	PHE	A	92	65.770	90.077	20.298	1.00	39.75	A
ATOM	343	CZ	PHE	A	92	64.756	90.550	19.456	1.00	39.75	A
ATOM	344	C	PHE	A	92	70.676	92.502	17.577	1.00	37.77	A
ATOM	345	O	PHE	A	92	70.695	93.728	17.569	1.00	37.77	A
ATOM	346	N	GLY	A	93	71.748	91.747	17.358	1.00	36.90	A
ATOM	347	CA	GLY	A	93	73.042	92.335	17.084	1.00	36.90	A
ATOM	348	C	GLY	A	93	73.276	92.459	15.587	1.00	36.90	A
ATOM	349	O	GLY	A	93	74.302	92.996	15.158	1.00	36.90	A
ATOM	350	N	ILE	A	94	72.337	91.958	14.784	1.00	32.21	A

FIGURE 2 Continued

ATOM	351	CA	ILE	A	94	72.472	92.053	13.342	1.00	32.21	A
ATOM	352	CB	ILE	A	94	71.706	90.905	12.633	1.00	31.38	A
ATOM	353	CG2	ILE	A	94	71.667	91.141	11.107	1.00	31.38	A
ATOM	354	CG1	ILE	A	94	72.414	89.581	12.958	1.00	31.38	A
ATOM	355	CD1	ILE	A	94	71.877	88.372	12.262	1.00	31.38	A
ATOM	356	C	ILE	A	94	71.962	93.431	12.934	1.00	32.21	A
ATOM	357	O	ILE	A	94	70.797	93.771	13.147	1.00	32.21	A
ATOM	358	N	LEU	A	95	72.854	94.224	12.351	1.00	35.55	A
ATOM	359	CA	LEU	A	95	72.535	95.596	11.982	1.00	35.55	A
ATOM	360	CB	LEU	A	95	73.436	96.543	12.790	1.00	30.56	A
ATOM	361	CG	LEU	A	95	73.724	96.086	14.230	1.00	30.56	A
ATOM	362	CD1	LEU	A	95	74.864	96.922	14.819	1.00	30.56	A
ATOM	363	CD2	LEU	A	95	72.451	96.186	15.089	1.00	30.56	A
ATOM	364	C	LEU	A	95	72.671	95.920	10.502	1.00	35.55	A
ATOM	365	O	LEU	A	95	73.285	95.179	9.733	1.00	35.55	A
ATOM	366	N	GLU	A	96	72.094	97.050	10.116	1.00	41.25	A
ATOM	367	CA	GLU	A	96	72.139	97.510	8.739	1.00	41.25	A
ATOM	368	CB	GLU	A	96	70.729	97.687	8.173	1.00	51.47	A
ATOM	369	CG	GLU	A	96	70.713	97.871	6.669	1.00	51.47	A
ATOM	370	CD	GLU	A	96	69.514	98.653	6.172	1.00	51.47	A
ATOM	371	OE1	GLU	A	96	68.391	98.423	6.670	1.00	51.47	A
ATOM	372	OE2	GLU	A	96	69.690	99.497	5.269	1.00	51.47	A
ATOM	373	C	GLU	A	96	72.827	98.860	8.751	1.00	41.25	A
ATOM	374	O	GLU	A	96	72.385	99.772	9.453	1.00	41.25	A
ATOM	375	N	PHE	A	97	73.913	98.991	7.995	1.00	39.56	A
ATOM	376	CA	PHE	A	97	74.609	100.267	7.948	1.00	39.56	A
ATOM	377	CB	PHE	A	97	76.115	100.063	7.831	1.00	37.09	A
ATOM	378	CG	PHE	A	97	76.810	99.968	9.157	1.00	37.09	A
ATOM	379	CD1	PHE	A	97	76.422	99.012	10.100	1.00	37.09	A
ATOM	380	CD2	PHE	A	97	77.850	100.838	9.471	1.00	37.09	A
ATOM	381	CE1	PHE	A	97	77.064	98.921	11.338	1.00	37.09	A
ATOM	382	CE2	PHE	A	97	78.505	100.759	10.710	1.00	37.09	A
ATOM	383	CZ	PHE	A	97	78.109	99.797	11.646	1.00	37.09	A
ATOM	384	C	PHE	A	97	74.101	101.133	6.808	1.00	39.56	A
ATOM	385	O	PHE	A	97	73.987	100.687	5.667	1.00	39.56	A
ATOM	386	N	ILE	A	98	73.787	102.379	7.133	1.00	45.56	A
ATOM	387	CA	ILE	A	98	73.279	103.309	6.147	1.00	45.56	A
ATOM	388	CB	ILE	A	98	71.864	103.776	6.529	1.00	42.37	A
ATOM	389	CG2	ILE	A	98	71.379	104.819	5.543	1.00	42.37	A
ATOM	390	CG1	ILE	A	98	70.925	102.565	6.564	1.00	42.37	A
ATOM	391	CD1	ILE	A	98	69.815	102.675	7.576	1.00	42.37	A
ATOM	392	C	ILE	A	98	74.197	104.510	6.042	1.00	45.56	A
ATOM	393	O	ILE	A	98	74.421	105.219	7.020	1.00	45.56	A
ATOM	394	N	SER	A	99	74.738	104.726	4.853	1.00	39.32	A
ATOM	395	CA	SER	A	99	75.622	105.848	4.607	1.00	39.32	A
ATOM	396	CB	SER	A	99	76.440	105.597	3.342	1.00	55.24	A
ATOM	397	OG	SER	A	99	77.208	106.737	2.999	1.00	55.24	A
ATOM	398	C	SER	A	99	74.770	107.104	4.436	1.00	39.32	A
ATOM	399	O	SER	A	99	73.955	107.188	3.514	1.00	39.32	A
ATOM	400	N	ILE	A	100	74.949	108.071	5.332	1.00	49.40	A
ATOM	401	CA	ILE	A	100	74.188	109.315	5.264	1.00	49.40	A
ATOM	402	CB	ILE	A	100	73.907	109.865	6.685	1.00	40.10	A
ATOM	403	CG2	ILE	A	100	73.193	111.209	6.595	1.00	40.10	A
ATOM	404	CG1	ILE	A	100	73.068	108.857	7.480	1.00	40.10	A
ATOM	405	CD1	ILE	A	100	71.660	108.634	6.933	1.00	40.10	A
ATOM	406	C	ILE	A	100	74.934	110.374	4.441	1.00	49.40	A
ATOM	407	O	ILE	A	100	74.324	111.168	3.723	1.00	49.40	A

FIGURE 2 Continued

ATOM	408	N	ALA	A	101	76.258	110.369	4.552	1.00	45.08	A
ATOM	409	CA	ALA	A	101	77.112	111.305	3.832	1.00	45.08	A
ATOM	410	CB	ALA	A	101	76.842	112.739	4.295	1.00	35.21	A
ATOM	411	C	ALA	A	101	78.545	110.907	4.140	1.00	45.08	A
ATOM	412	O	ALA	A	101	78.770	109.913	4.822	1.00	45.08	A
ATOM	413	N	VAL	A	102	79.518	111.663	3.649	1.00	46.06	A
ATOM	414	CA	VAL	A	102	80.907	111.317	3.923	1.00	46.06	A
ATOM	415	CB	VAL	A	102	81.895	112.255	3.178	1.00	47.26	A
ATOM	416	CG1	VAL	A	102	83.329	111.816	3.452	1.00	47.26	A
ATOM	417	CG2	VAL	A	102	81.612	112.237	1.676	1.00	47.26	A
ATOM	418	C	VAL	A	102	81.205	111.397	5.421	1.00	46.06	A
ATOM	419	O	VAL	A	102	81.063	112.456	6.035	1.00	46.06	A
ATOM	420	N	GLY	A	103	81.610	110.268	6.000	1.00	36.05	A
ATOM	421	CA	GLY	A	103	81.938	110.219	7.414	1.00	36.05	A
ATOM	422	C	GLY	A	103	80.764	110.052	8.359	1.00	36.05	A
ATOM	423	O	GLY	A	103	80.955	110.004	9.571	1.00	36.05	A
ATOM	424	N	LEU	A	104	79.550	109.963	7.827	1.00	42.00	A
ATOM	425	CA	LEU	A	104	78.367	109.816	8.675	1.00	42.00	A
ATOM	426	CB	LEU	A	104	77.425	111.019	8.526	1.00	39.82	A
ATOM	427	CG	LEU	A	104	77.926	112.428	8.858	1.00	39.82	A
ATOM	428	CD1	LEU	A	104	76.782	113.414	8.649	1.00	39.82	A
ATOM	429	CD2	LEU	A	104	78.435	112.492	10.297	1.00	39.82	A
ATOM	430	C	LEU	A	104	77.589	108.562	8.334	1.00	42.00	A
ATOM	431	O	LEU	A	104	77.488	108.168	7.170	1.00	42.00	A
ATOM	432	N	VAL	A	105	77.018	107.939	9.352	1.00	39.38	A
ATOM	433	CA	VAL	A	105	76.251	106.740	9.116	1.00	39.38	A
ATOM	434	CB	VAL	A	105	77.105	105.476	9.327	1.00	33.62	A
ATOM	435	CG1	VAL	A	105	78.323	105.503	8.416	1.00	33.62	A
ATOM	436	CG2	VAL	A	105	77.531	105.393	10.793	1.00	33.62	A
ATOM	437	C	VAL	A	105	75.072	106.645	10.055	1.00	39.38	A
ATOM	438	O	VAL	A	105	74.956	107.392	11.032	1.00	39.38	A
ATOM	439	N	SER	A	106	74.190	105.713	9.728	1.00	38.61	A
ATOM	440	CA	SER	A	106	73.029	105.416	10.539	1.00	38.61	A
ATOM	441	CB	SER	A	106	71.750	105.863	9.845	1.00	57.92	A
ATOM	442	OG	SER	A	106	71.640	107.272	9.908	1.00	57.92	A
ATOM	443	C	SER	A	106	73.076	103.901	10.703	1.00	38.61	A
ATOM	444	O	SER	A	106	73.497	103.182	9.805	1.00	38.61	A
ATOM	445	N	ILE	A	107	72.660	103.428	11.863	1.00	37.16	A
ATOM	446	CA	ILE	A	107	72.693	102.018	12.159	1.00	37.16	A
ATOM	447	CB	ILE	A	107	73.662	101.759	13.323	1.00	29.59	A
ATOM	448	CG2	ILE	A	107	73.694	100.285	13.658	1.00	29.59	A
ATOM	449	CG1	ILE	A	107	75.054	102.280	12.939	1.00	29.59	A
ATOM	450	CD1	ILE	A	107	76.061	102.269	14.068	1.00	29.59	A
ATOM	451	C	ILE	A	107	71.304	101.535	12.521	1.00	37.16	A
ATOM	452	O	ILE	A	107	70.704	102.012	13.478	1.00	37.16	A
ATOM	453	N	ARG	A	108	70.807	100.570	11.755	1.00	46.61	A
ATOM	454	CA	ARG	A	108	69.485	100.029	11.989	1.00	46.61	A
ATOM	455	CB	ARG	A	108	68.654	100.169	10.725	1.00	57.86	A
ATOM	456	CG	ARG	A	108	67.182	100.039	10.982	1.00	57.86	A
ATOM	457	CD	ARG	A	108	66.395	100.077	9.706	1.00	57.86	A
ATOM	458	NE	ARG	A	108	64.978	100.261	9.982	1.00	57.86	A
ATOM	459	CZ	ARG	A	108	64.012	100.019	9.104	1.00	57.86	A
ATOM	460	NH1	ARG	A	108	64.317	99.575	7.890	1.00	57.86	A
ATOM	461	NH2	ARG	A	108	62.745	100.230	9.437	1.00	57.86	A
ATOM	462	C	ARG	A	108	69.484	98.564	12.434	1.00	46.61	A
ATOM	463	O	ARG	A	108	70.154	97.722	11.836	1.00	46.61	A
ATOM	464	N	GLY	A	109	68.736	98.269	13.498	1.00	40.40	A

FIGURE 2 Continued

ATOM	465	CA	GLY	A	109	68.637	96.903	13.968	1.00	40.40	A
ATOM	466	C	GLY	A	109	67.728	96.209	12.969	1.00	40.40	A
ATOM	467	O	GLY	A	109	66.565	96.600	12.800	1.00	40.40	A
ATOM	468	N	VAL	A	110	68.251	95.196	12.282	1.00	36.06	A
ATOM	469	CA	VAL	A	110	67.460	94.495	11.288	1.00	36.06	A
ATOM	470	CB	VAL	A	110	68.275	93.377	10.602	1.00	32.16	A
ATOM	471	CG1	VAL	A	110	67.360	92.538	9.711	1.00	32.16	A
ATOM	472	CG2	VAL	A	110	69.395	93.995	9.762	1.00	32.16	A
ATOM	473	C	VAL	A	110	66.194	93.894	11.876	1.00	36.06	A
ATOM	474	O	VAL	A	110	65.109	94.124	11.363	1.00	36.06	A
ATOM	475	N	ASP	A	111	66.344	93.140	12.958	1.00	47.90	A
ATOM	476	CA	ASP	A	111	65.218	92.484	13.600	1.00	47.90	A
ATOM	477	CB	ASP	A	111	65.718	91.522	14.661	1.00	65.18	A
ATOM	478	CG	ASP	A	111	64.738	90.420	14.938	1.00	65.18	A
ATOM	479	OD1	ASP	A	111	64.911	89.316	14.379	1.00	65.18	A
ATOM	480	OD2	ASP	A	111	63.785	90.661	15.701	1.00	65.18	A
ATOM	481	C	ASP	A	111	64.221	93.438	14.241	1.00	47.90	A
ATOM	482	O	ASP	A	111	63.016	93.295	14.050	1.00	47.90	A
ATOM	483	N	SER	A	112	64.716	94.402	15.011	1.00	48.62	A
ATOM	484	CA	SER	A	112	63.841	95.361	15.679	1.00	48.62	A
ATOM	485	CB	SER	A	112	64.578	96.067	16.824	1.00	41.51	A
ATOM	486	OG	SER	A	112	65.442	97.079	16.329	1.00	41.51	A
ATOM	487	C	SER	A	112	63.301	96.419	14.728	1.00	48.62	A
ATOM	488	O	SER	A	112	62.207	96.937	14.930	1.00	48.62	A
ATOM	489	N	GLY	A	113	64.072	96.744	13.697	1.00	36.94	A
ATOM	490	CA	GLY	A	113	63.647	97.766	12.760	1.00	36.94	A
ATOM	491	C	GLY	A	113	63.984	99.148	13.302	1.00	36.94	A
ATOM	492	O	GLY	A	113	63.781	100.156	12.620	1.00	36.94	A
ATOM	493	N	LEU	A	114	64.520	99.197	14.521	1.00	42.02	A
ATOM	494	CA	LEU	A	114	64.871	100.463	15.159	1.00	42.02	A
ATOM	495	CB	LEU	A	114	64.736	100.334	16.679	1.00	31.99	A
ATOM	496	CG	LEU	A	114	63.376	99.778	17.130	1.00	31.99	A
ATOM	497	CD1	LEU	A	114	63.406	99.447	18.612	1.00	31.99	A
ATOM	498	CD2	LEU	A	114	62.277	100.788	16.795	1.00	31.99	A
ATOM	499	C	LEU	A	114	66.268	100.986	14.819	1.00	42.02	A
ATOM	500	O	LEU	A	114	67.215	100.220	14.624	1.00	42.02	A
ATOM	501	N	TYR	A	115	66.374	102.308	14.742	1.00	41.73	A
ATOM	502	CA	TYR	A	115	67.632	102.977	14.449	1.00	41.73	A
ATOM	503	CB	TYR	A	115	67.373	104.276	13.690	1.00	43.44	A
ATOM	504	CG	TYR	A	115	66.723	104.072	12.355	1.00	43.44	A
ATOM	505	CD1	TYR	A	115	67.485	103.750	11.234	1.00	43.44	A
ATOM	506	CE1	TYR	A	115	66.886	103.512	10.007	1.00	43.44	A
ATOM	507	CD2	TYR	A	115	65.336	104.156	12.214	1.00	43.44	A
ATOM	508	CE2	TYR	A	115	64.723	103.919	10.991	1.00	43.44	A
ATOM	509	CZ	TYR	A	115	65.505	103.596	9.893	1.00	43.44	A
ATOM	510	OH	TYR	A	115	64.915	103.333	8.680	1.00	43.44	A
ATOM	511	C	TYR	A	115	68.350	103.312	15.748	1.00	41.73	A
ATOM	512	O	TYR	A	115	67.719	103.670	16.747	1.00	41.73	A
ATOM	513	N	LEU	A	116	69.669	103.183	15.739	1.00	33.73	A
ATOM	514	CA	LEU	A	116	70.441	103.525	16.916	1.00	33.73	A
ATOM	515	CB	LEU	A	116	71.898	103.106	16.759	1.00	33.45	A
ATOM	516	CG	LEU	A	116	72.749	103.390	17.999	1.00	33.45	A
ATOM	517	CD1	LEU	A	116	72.195	102.589	19.172	1.00	33.45	A
ATOM	518	CD2	LEU	A	116	74.211	103.027	17.743	1.00	33.45	A
ATOM	519	C	LEU	A	116	70.374	105.045	17.034	1.00	33.73	A
ATOM	520	O	LEU	A	116	70.591	105.774	16.053	1.00	33.73	A
ATOM	521	N	GLY	A	117	70.048	105.522	18.232	1.00	33.61	A

FIGURE 2 Continued

ATOM	522	CA	GLY	A	117	69.981	106.953	18.455	1.00	33.61	A
ATOM	523	C	GLY	A	117	70.658	107.316	19.759	1.00	33.61	A
ATOM	524	O	GLY	A	117	70.848	106.470	20.635	1.00	33.61	A
ATOM	525	N	MET	A	118	71.065	108.570	19.879	1.00	30.89	A
ATOM	526	CA	MET	A	118	71.665	109.040	21.119	1.00	30.89	A
ATOM	527	CB	MET	A	118	73.166	109.277	20.977	1.00	36.59	A
ATOM	528	CG	MET	A	118	73.830	109.497	22.329	1.00	36.59	A
ATOM	529	SD	MET	A	118	75.518	110.087	22.258	1.00	36.59	A
ATOM	530	CE	MET	A	118	76.443	108.534	22.088	1.00	36.59	A
ATOM	531	C	MET	A	118	70.967	110.348	21.441	1.00	30.89	A
ATOM	532	O	MET	A	118	71.003	111.288	20.644	1.00	30.89	A
ATOM	533	N	ASN	A	119	70.308	110.413	22.590	1.00	44.08	A
ATOM	534	CA	ASN	A	119	69.614	111.645	22.944	1.00	44.08	A
ATOM	535	CB	ASN	A	119	68.437	111.354	23.881	1.00	34.21	A
ATOM	536	CG	ASN	A	119	68.874	110.847	25.233	1.00	34.21	A
ATOM	537	OD1	ASN	A	119	70.030	111.020	25.642	1.00	34.21	A
ATOM	538	ND2	ASN	A	119	67.947	110.229	25.954	1.00	34.21	A
ATOM	539	C	ASN	A	119	70.566	112.677	23.572	1.00	44.08	A
ATOM	540	O	ASN	A	119	71.746	112.398	23.800	1.00	44.08	A
ATOM	541	N	GLU	A	120	70.037	113.867	23.838	1.00	49.84	A
ATOM	542	CA	GLU	A	120	70.804	114.965	24.412	1.00	49.84	A
ATOM	543	CB	GLU	A	120	69.861	116.142	24.648	1.00	71.86	A
ATOM	544	CG	GLU	A	120	70.538	117.446	24.987	1.00	71.86	A
ATOM	545	CD	GLU	A	120	69.752	118.639	24.473	1.00	71.86	A
ATOM	546	OE1	GLU	A	120	68.519	118.677	24.688	1.00	71.86	A
ATOM	547	OE2	GLU	A	120	70.369	119.535	23.856	1.00	71.86	A
ATOM	548	C	GLU	A	120	71.580	114.618	25.695	1.00	49.84	A
ATOM	549	O	GLU	A	120	72.625	115.204	25.964	1.00	49.84	A
ATOM	550	N	LYS	A	121	71.081	113.670	26.483	1.00	46.92	A
ATOM	551	CA	LYS	A	121	71.771	113.267	27.707	1.00	46.92	A
ATOM	552	CB	LYS	A	121	70.806	112.604	28.692	1.00	54.84	A
ATOM	553	CG	LYS	A	121	69.660	113.476	29.163	1.00	54.84	A
ATOM	554	CD	LYS	A	121	68.682	112.679	30.023	1.00	54.84	A
ATOM	555	CE	LYS	A	121	67.455	113.512	30.366	1.00	54.84	A
ATOM	556	NZ	LYS	A	121	66.380	112.716	31.028	1.00	54.84	A
ATOM	557	C	LYS	A	121	72.875	112.268	27.378	1.00	46.92	A
ATOM	558	O	LYS	A	121	73.559	111.775	28.275	1.00	46.92	A
ATOM	559	N	GLY	A	122	73.026	111.953	26.093	1.00	43.12	A
ATOM	560	CA	GLY	A	122	74.044	111.008	25.670	1.00	43.12	A
ATOM	561	C	GLY	A	122	73.627	109.557	25.824	1.00	43.12	A
ATOM	562	O	GLY	A	122	74.454	108.649	25.737	1.00	43.12	A
ATOM	563	N	GLU	A	123	72.344	109.318	26.051	1.00	41.94	A
ATOM	564	CA	GLU	A	123	71.888	107.946	26.214	1.00	41.94	A
ATOM	565	CB	GLU	A	123	70.700	107.887	27.178	1.00	66.72	A
ATOM	566	CG	GLU	A	123	71.046	108.284	28.605	1.00	66.72	A
ATOM	567	CD	GLU	A	123	69.906	108.036	29.578	1.00	66.72	A
ATOM	568	OE1	GLU	A	123	68.828	108.658	29.416	1.00	66.72	A
ATOM	569	OE2	GLU	A	123	70.098	107.213	30.501	1.00	66.72	A
ATOM	570	C	GLU	A	123	71.516	107.306	24.881	1.00	41.94	A
ATOM	571	O	GLU	A	123	70.896	107.940	24.018	1.00	41.94	A
ATOM	572	N	LEU	A	124	71.926	106.050	24.719	1.00	42.10	A
ATOM	573	CA	LEU	A	124	71.636	105.294	23.511	1.00	42.10	A
ATOM	574	CB	LEU	A	124	72.618	104.126	23.359	1.00	31.10	A
ATOM	575	CG	LEU	A	124	74.101	104.456	23.275	1.00	31.10	A
ATOM	576	CD1	LEU	A	124	74.905	103.164	23.248	1.00	31.10	A
ATOM	577	CD2	LEU	A	124	74.357	105.307	22.042	1.00	31.10	A
ATOM	578	C	LEU	A	124	70.227	104.729	23.620	1.00	42.10	A

FIGURE 2 Continued

ATOM	579	O	LEU	A	124	69.794	104.328	24.701	1.00	42.10	A
ATOM	580	N	TYR	A	125	69.521	104.688	22.499	1.00	35.83	A
ATOM	581	CA	TYR	A	125	68.172	104.144	22.483	1.00	35.83	A
ATOM	582	CB	TYR	A	125	67.162	105.191	22.969	1.00	33.16	A
ATOM	583	CG	TYR	A	125	66.998	106.361	22.027	1.00	33.16	A
ATOM	584	CD1	TYR	A	125	67.900	107.429	22.035	1.00	33.16	A
ATOM	585	CE1	TYR	A	125	67.761	108.503	21.151	1.00	33.16	A
ATOM	586	CD2	TYR	A	125	65.951	106.392	21.111	1.00	33.16	A
ATOM	587	CE2	TYR	A	125	65.798	107.451	20.227	1.00	33.16	A
ATOM	588	CZ	TYR	A	125	66.705	108.506	20.251	1.00	33.16	A
ATOM	589	OH	TYR	A	125	66.521	109.560	19.378	1.00	33.16	A
ATOM	590	C	TYR	A	125	67.827	103.726	21.063	1.00	35.83	A
ATOM	591	O	TYR	A	125	68.450	104.188	20.110	1.00	35.83	A
ATOM	592	N	GLY	A	126	66.836	102.851	20.928	1.00	38.80	A
ATOM	593	CA	GLY	A	126	66.420	102.405	19.615	1.00	38.80	A
ATOM	594	C	GLY	A	126	65.299	103.311	19.162	1.00	38.80	A
ATOM	595	O	GLY	A	126	64.254	103.360	19.809	1.00	38.80	A
ATOM	596	N	SER	A	127	65.512	104.023	18.055	1.00	42.59	A
ATOM	597	CA	SER	A	127	64.527	104.960	17.525	1.00	42.59	A
ATOM	598	CB	SER	A	127	65.234	106.231	17.054	1.00	44.81	A
ATOM	599	OG	SER	A	127	64.333	107.119	16.413	1.00	44.81	A
ATOM	600	C	SER	A	127	63.653	104.438	16.388	1.00	42.59	A
ATOM	601	O	SER	A	127	64.138	103.859	15.415	1.00	42.59	A
ATOM	602	N	GLU	A	128	62.353	104.681	16.508	1.00	48.10	A
ATOM	603	CA	GLU	A	128	61.400	104.268	15.498	1.00	48.10	A
ATOM	604	CB	GLU	A	128	59.991	104.662	15.924	1.00	100.00	A
ATOM	605	CG	GLU	A	128	58.916	104.165	14.989	1.00	100.00	A
ATOM	606	CD	GLU	A	128	57.575	104.803	15.267	1.00	100.00	A
ATOM	607	OE1	GLU	A	128	57.432	106.021	15.012	1.00	100.00	A
ATOM	608	OE2	GLU	A	128	56.669	104.089	15.744	1.00	100.00	A
ATOM	609	C	GLU	A	128	61.729	104.924	14.155	1.00	48.10	A
ATOM	610	O	GLU	A	128	61.665	104.280	13.110	1.00	48.10	A
ATOM	611	N	LYS	A	129	62.094	106.203	14.186	1.00	46.49	A
ATOM	612	CA	LYS	A	129	62.410	106.925	12.961	1.00	46.49	A
ATOM	613	CB	LYS	A	129	61.486	108.135	12.824	1.00	97.04	A
ATOM	614	CG	LYS	A	129	60.019	107.755	12.789	1.00	97.04	A
ATOM	615	CD	LYS	A	129	59.136	108.939	12.463	1.00	97.04	A
ATOM	616	CE	LYS	A	129	57.675	108.521	12.392	1.00	97.04	A
ATOM	617	NZ	LYS	A	129	56.788	109.657	12.008	1.00	97.04	A
ATOM	618	C	LYS	A	129	63.864	107.376	12.853	1.00	46.49	A
ATOM	619	O	LYS	A	129	64.523	107.669	13.853	1.00	46.49	A
ATOM	620	N	LEU	A	130	64.367	107.422	11.626	1.00	48.47	A
ATOM	621	CA	LEU	A	130	65.736	107.851	11.409	1.00	48.47	A
ATOM	622	CB	LEU	A	130	66.228	107.398	10.033	1.00	48.95	A
ATOM	623	CG	LEU	A	130	67.754	107.322	9.880	1.00	48.95	A
ATOM	624	CD1	LEU	A	130	68.079	106.741	8.507	1.00	48.95	A
ATOM	625	CD2	LEU	A	130	68.399	108.695	10.054	1.00	48.95	A
ATOM	626	C	LEU	A	130	65.765	109.378	11.525	1.00	48.47	A
ATOM	627	O	LEU	A	130	65.411	110.101	10.593	1.00	48.47	A
ATOM	628	N	THR	A	131	66.194	109.858	12.686	1.00	40.24	A
ATOM	629	CA	THR	A	131	66.245	111.285	12.946	1.00	40.24	A
ATOM	630	CB	THR	A	131	65.458	111.627	14.235	1.00	40.73	A
ATOM	631	OG1	THR	A	131	66.038	110.940	15.358	1.00	40.73	A
ATOM	632	CG2	THR	A	131	64.000	111.194	14.090	1.00	40.73	A
ATOM	633	C	THR	A	131	67.669	111.792	13.085	1.00	40.24	A
ATOM	634	O	THR	A	131	68.628	111.042	12.916	1.00	40.24	A
ATOM	635	N	GLN	A	132	67.792	113.079	13.390	1.00	50.95	A

FIGURE 2 Continued

ATOM	636	CA	GLN	A	132	69.093	113.700	13.556	1.00	50.95	A
ATOM	637	CB	GLN	A	132	68.932	115.198	13.808	1.00	96.26	A
ATOM	638	CG	GLN	A	132	68.197	115.916	12.690	1.00	96.26	A
ATOM	639	CD	GLN	A	132	68.895	115.780	11.344	1.00	96.26	A
ATOM	640	OE1	GLN	A	132	69.184	114.673	10.888	1.00	96.26	A
ATOM	641	NE2	GLN	A	132	69.162	116.910	10.698	1.00	96.26	A
ATOM	642	C	GLN	A	132	69.859	113.046	14.694	1.00	50.95	A
ATOM	643	O	GLN	A	132	71.087	113.018	14.676	1.00	50.95	A
ATOM	644	N	GLU	A	133	69.142	112.509	15.679	1.00	38.78	A
ATOM	645	CA	GLU	A	133	69.802	111.845	16.802	1.00	38.78	A
ATOM	646	CB	GLU	A	133	68.849	111.697	17.995	1.00	42.92	A
ATOM	647	CG	GLU	A	133	68.371	112.986	18.628	1.00	42.92	A
ATOM	648	CD	GLU	A	133	67.837	112.767	20.042	1.00	42.92	A
ATOM	649	OE1	GLU	A	133	67.334	111.662	20.330	1.00	42.92	A
ATOM	650	OE2	GLU	A	133	67.915	113.699	20.870	1.00	42.92	A
ATOM	651	C	GLU	A	133	70.285	110.447	16.392	1.00	38.78	A
ATOM	652	O	GLU	A	133	70.805	109.693	17.211	1.00	38.78	A
ATOM	653	N	CYS	A	134	70.110	110.112	15.122	1.00	37.59	A
ATOM	654	CA	CYS	A	134	70.486	108.803	14.625	1.00	37.59	A
ATOM	655	CB	CYS	A	134	69.264	108.133	14.011	1.00	44.56	A
ATOM	656	SG	CYS	A	134	67.933	107.967	15.181	1.00	44.56	A
ATOM	657	C	CYS	A	134	71.614	108.828	13.616	1.00	37.59	A
ATOM	658	O	CYS	A	134	71.873	107.834	12.944	1.00	37.59	A
ATOM	659	N	VAL	A	135	72.275	109.967	13.502	1.00	43.83	A
ATOM	660	CA	VAL	A	135	73.380	110.092	12.575	1.00	43.83	A
ATOM	661	CB	VAL	A	135	73.245	111.373	11.719	1.00	31.92	A
ATOM	662	CG1	VAL	A	135	74.511	111.605	10.910	1.00	31.92	A
ATOM	663	CG2	VAL	A	135	72.040	111.239	10.781	1.00	31.92	A
ATOM	664	C	VAL	A	135	74.657	110.135	13.392	1.00	43.83	A
ATOM	665	O	VAL	A	135	74.797	110.964	14.295	1.00	43.83	A
ATOM	666	N	PHE	A	136	75.580	109.225	13.094	1.00	36.43	A
ATOM	667	CA	PHE	A	136	76.834	109.183	13.823	1.00	36.43	A
ATOM	668	CB	PHE	A	136	76.995	107.856	14.550	1.00	27.81	A
ATOM	669	CG	PHE	A	136	75.917	107.588	15.537	1.00	27.81	A
ATOM	670	CD1	PHE	A	136	74.694	107.063	15.123	1.00	27.81	A
ATOM	671	CD2	PHE	A	136	76.096	107.902	16.881	1.00	27.81	A
ATOM	672	CE1	PHE	A	136	73.654	106.852	16.034	1.00	27.81	A
ATOM	673	CE2	PHE	A	136	75.066	107.697	17.803	1.00	27.81	A
ATOM	674	CZ	PHE	A	136	73.838	107.170	17.378	1.00	27.81	A
ATOM	675	C	PHE	A	136	78.034	109.395	12.948	1.00	36.43	A
ATOM	676	O	PHE	A	136	78.054	108.995	11.785	1.00	36.43	A
ATOM	677	N	ARG	A	137	79.035	110.046	13.526	1.00	37.38	A
ATOM	678	CA	ARG	A	137	80.279	110.300	12.836	1.00	37.38	A
ATOM	679	CB	ARG	A	137	81.011	111.467	13.477	1.00	41.52	A
ATOM	680	CG	ARG	A	137	80.228	112.737	13.464	1.00	41.52	A
ATOM	681	CD	ARG	A	137	81.045	113.863	14.017	1.00	41.52	A
ATOM	682	NE	ARG	A	137	80.368	115.130	13.782	1.00	41.52	A
ATOM	683	CZ	ARG	A	137	80.944	116.319	13.916	1.00	41.52	A
ATOM	684	NH1	ARG	A	137	82.217	116.406	14.286	1.00	41.52	A
ATOM	685	NH2	ARG	A	137	80.246	117.416	13.673	1.00	41.52	A
ATOM	686	C	ARG	A	137	81.133	109.053	12.965	1.00	37.38	A
ATOM	687	O	ARG	A	137	81.595	108.704	14.066	1.00	37.38	A
ATOM	688	N	GLU	A	138	81.327	108.368	11.846	1.00	39.12	A
ATOM	689	CA	GLU	A	138	82.143	107.167	11.834	1.00	39.12	A
ATOM	690	CB	GLU	A	138	81.585	106.167	10.830	1.00	38.56	A
ATOM	691	CG	GLU	A	138	82.370	104.863	10.719	1.00	38.56	A
ATOM	692	CD	GLU	A	138	81.719	103.908	9.738	1.00	38.56	A

FIGURE 2 Continued

ATOM	693	OE1	GLU	A	138	81.670	104.249	8.542	1.00	38.56	A
ATOM	694	OE2	GLU	A	138	81.237	102.836	10.158	1.00	38.56	A
ATOM	695	C	GLU	A	138	83.560	107.567	11.451	1.00	39.12	A
ATOM	696	O	GLU	A	138	83.794	108.086	10.365	1.00	39.12	A
ATOM	697	N	GLN	A	139	84.499	107.334	12.357	1.00	40.20	A
ATOM	698	CA	GLN	A	139	85.893	107.671	12.113	1.00	40.20	A
ATOM	699	CB	GLN	A	139	86.253	108.971	12.816	1.00	41.33	A
ATOM	700	CG	GLN	A	139	85.593	110.190	12.243	1.00	41.33	A
ATOM	701	CD	GLN	A	139	85.751	111.386	13.150	1.00	41.33	A
ATOM	702	OE1	GLN	A	139	86.621	111.404	14.031	1.00	41.33	A
ATOM	703	NE2	GLN	A	139	84.920	112.399	12.940	1.00	41.33	A
ATOM	704	C	GLN	A	139	86.839	106.577	12.585	1.00	40.20	A
ATOM	705	O	GLN	A	139	86.724	106.082	13.706	1.00	40.20	A
ATOM	706	N	PHE	A	140	87.777	106.217	11.712	1.00	36.98	A
ATOM	707	CA	PHE	A	140	88.777	105.200	11.994	1.00	36.98	A
ATOM	708	CB	PHE	A	140	89.817	105.178	10.865	1.00	40.09	A
ATOM	709	CG	PHE	A	140	90.886	104.134	11.041	1.00	40.09	A
ATOM	710	CD1	PHE	A	140	91.951	104.347	11.914	1.00	40.09	A
ATOM	711	CD2	PHE	A	140	90.809	102.919	10.355	1.00	40.09	A
ATOM	712	CE1	PHE	A	140	92.924	103.364	12.104	1.00	40.09	A
ATOM	713	CE2	PHE	A	140	91.773	101.930	10.537	1.00	40.09	A
ATOM	714	CZ	PHE	A	140	92.834	102.150	11.412	1.00	40.09	A
ATOM	715	C	PHE	A	140	89.465	105.481	13.325	1.00	36.98	A
ATOM	716	O	PHE	A	140	89.768	106.626	13.644	1.00	36.98	A
ATOM	717	N	GLU	A	141	89.713	104.432	14.096	1.00	41.49	A
ATOM	718	CA	GLU	A	141	90.373	104.574	15.382	1.00	41.49	A
ATOM	719	CB	GLU	A	141	89.423	104.141	16.501	1.00	39.52	A
ATOM	720	CG	GLU	A	141	90.011	104.126	17.911	1.00	39.52	A
ATOM	721	CD	GLU	A	141	90.582	105.469	18.368	1.00	39.52	A
ATOM	722	OE1	GLU	A	141	90.166	106.531	17.844	1.00	39.52	A
ATOM	723	OE2	GLU	A	141	91.446	105.456	19.274	1.00	39.52	A
ATOM	724	C	GLU	A	141	91.642	103.727	15.392	1.00	41.49	A
ATOM	725	O	GLU	A	141	92.739	104.239	15.590	1.00	41.49	A
ATOM	726	N	GLU	A	142	91.492	102.432	15.157	1.00	46.79	A
ATOM	727	CA	GLU	A	142	92.636	101.536	15.152	1.00	46.79	A
ATOM	728	CB	GLU	A	142	93.272	101.483	16.546	1.00	60.39	A
ATOM	729	CG	GLU	A	142	92.300	101.193	17.701	1.00	60.39	A
ATOM	730	CD	GLU	A	142	92.138	99.703	18.029	1.00	60.39	A
ATOM	731	OE1	GLU	A	142	92.916	98.880	17.497	1.00	60.39	A
ATOM	732	OE2	GLU	A	142	91.236	99.361	18.835	1.00	60.39	A
ATOM	733	C	GLU	A	142	92.241	100.139	14.717	1.00	46.79	A
ATOM	734	O	GLU	A	142	91.230	99.607	15.167	1.00	46.79	A
ATOM	735	N	ASN	A	143	93.040	99.558	13.827	1.00	37.61	A
ATOM	736	CA	ASN	A	143	92.800	98.205	13.336	1.00	37.61	A
ATOM	737	CB	ASN	A	143	93.074	97.208	14.448	1.00	36.68	A
ATOM	738	CG	ASN	A	143	94.527	97.204	14.856	1.00	36.68	A
ATOM	739	OD1	ASN	A	143	95.405	96.922	14.036	1.00	36.68	A
ATOM	740	ND2	ASN	A	143	94.796	97.526	16.115	1.00	36.68	A
ATOM	741	C	ASN	A	143	91.406	97.995	12.790	1.00	37.61	A
ATOM	742	O	ASN	A	143	90.827	96.921	12.940	1.00	37.61	A
ATOM	743	N	TRP	A	144	90.881	99.037	12.156	1.00	33.61	A
ATOM	744	CA	TRP	A	144	89.558	99.024	11.555	1.00	33.61	A
ATOM	745	CB	TRP	A	144	89.422	97.825	10.611	1.00	35.86	A
ATOM	746	CG	TRP	A	144	90.430	97.988	9.550	1.00	35.86	A
ATOM	747	CD2	TRP	A	144	90.500	99.070	8.619	1.00	35.86	A
ATOM	748	CE2	TRP	A	144	91.741	98.969	7.957	1.00	35.86	A
ATOM	749	CE3	TRP	A	144	89.637	100.125	8.287	1.00	35.86	A

FIGURE 2 Continued

ATOM	750	CD1	TRP	A	144	91.595	97.283	9.406	1.00	35.86	A
ATOM	751	NE1	TRP	A	144	92.384	97.868	8.458	1.00	35.86	A
ATOM	752	CZ2	TRP	A	144	92.146	99.889	6.976	1.00	35.86	A
ATOM	753	CZ3	TRP	A	144	90.034	101.039	7.315	1.00	35.86	A
ATOM	754	CH2	TRP	A	144	91.280	100.914	6.671	1.00	35.86	A
ATOM	755	C	TRP	A	144	88.401	99.132	12.529	1.00	33.61	A
ATOM	756	O	TRP	A	144	87.238	98.996	12.149	1.00	33.61	A
ATOM	757	N	TYR	A	145	88.729	99.354	13.795	1.00	36.97	A
ATOM	758	CA	TYR	A	145	87.692	99.613	14.774	1.00	36.97	A
ATOM	759	CB	TYR	A	145	88.187	99.470	16.202	1.00	39.02	A
ATOM	760	CG	TYR	A	145	88.164	98.077	16.739	1.00	39.02	A
ATOM	761	CD1	TYR	A	145	89.246	97.222	16.559	1.00	39.02	A
ATOM	762	CE1	TYR	A	145	89.242	95.951	17.104	1.00	39.02	A
ATOM	763	CD2	TYR	A	145	87.072	97.622	17.468	1.00	39.02	A
ATOM	764	CE2	TYR	A	145	87.055	96.355	18.013	1.00	39.02	A
ATOM	765	CZ	TYR	A	145	88.143	95.526	17.834	1.00	39.02	A
ATOM	766	OH	TYR	A	145	88.139	94.293	18.424	1.00	39.02	A
ATOM	767	C	TYR	A	145	87.448	101.100	14.543	1.00	36.97	A
ATOM	768	O	TYR	A	145	88.385	101.850	14.266	1.00	36.97	A
ATOM	769	N	ASN	A	146	86.203	101.530	14.623	1.00	32.33	A
ATOM	770	CA	ASN	A	146	85.924	102.941	14.463	1.00	32.33	A
ATOM	771	CB	ASN	A	146	84.869	103.184	13.381	1.00	40.35	A
ATOM	772	CG	ASN	A	146	85.298	102.693	12.022	1.00	40.35	A
ATOM	773	OD1	ASN	A	146	86.365	103.058	11.528	1.00	40.35	A
ATOM	774	ND2	ASN	A	146	84.464	101.870	11.400	1.00	40.35	A
ATOM	775	C	ASN	A	146	85.372	103.429	15.786	1.00	32.33	A
ATOM	776	O	ASN	A	146	85.229	102.674	16.753	1.00	32.33	A
ATOM	777	N	THR	A	147	85.095	104.720	15.825	1.00	30.02	A
ATOM	778	CA	THR	A	147	84.465	105.330	16.975	1.00	30.02	A
ATOM	779	CB	THR	A	147	85.303	106.456	17.602	1.00	33.62	A
ATOM	780	OG1	THR	A	147	85.681	107.402	16.593	1.00	33.62	A
ATOM	781	CG2	THR	A	147	86.530	105.882	18.284	1.00	33.62	A
ATOM	782	C	THR	A	147	83.251	105.921	16.301	1.00	30.02	A
ATOM	783	O	THR	A	147	83.298	106.263	15.114	1.00	30.02	A
ATOM	784	N	TYR	A	148	82.153	105.993	17.038	1.00	41.03	A
ATOM	785	CA	TYR	A	148	80.929	106.559	16.503	1.00	41.03	A
ATOM	786	CB	TYR	A	148	79.875	105.461	16.317	1.00	34.61	A
ATOM	787	CG	TYR	A	148	80.270	104.413	15.295	1.00	34.61	A
ATOM	788	CD1	TYR	A	148	81.178	103.405	15.617	1.00	34.61	A
ATOM	789	CE1	TYR	A	148	81.605	102.480	14.659	1.00	34.61	A
ATOM	790	CD2	TYR	A	148	79.787	104.470	13.989	1.00	34.61	A
ATOM	791	CE2	TYR	A	148	80.199	103.562	13.025	1.00	34.61	A
ATOM	792	CZ	TYR	A	148	81.113	102.569	13.359	1.00	34.61	A
ATOM	793	OH	TYR	A	148	81.571	101.697	12.393	1.00	34.61	A
ATOM	794	C	TYR	A	148	80.451	107.620	17.476	1.00	41.03	A
ATOM	795	O	TYR	A	148	80.125	107.324	18.632	1.00	41.03	A
ATOM	796	N	SER	A	149	80.428	108.865	17.019	1.00	37.11	A
ATOM	797	CA	SER	A	149	79.988	109.950	17.889	1.00	37.11	A
ATOM	798	CB	SER	A	149	81.093	111.002	18.051	1.00	35.33	A
ATOM	799	OG	SER	A	149	81.377	111.642	16.815	1.00	35.33	A
ATOM	800	C	SER	A	149	78.744	110.608	17.341	1.00	37.11	A
ATOM	801	O	SER	A	149	78.483	110.568	16.133	1.00	37.11	A
ATOM	802	N	SER	A	150	77.969	111.200	18.241	1.00	33.63	A
ATOM	803	CA	SER	A	150	76.758	111.890	17.842	1.00	33.63	A
ATOM	804	CB	SER	A	150	76.061	112.463	19.073	1.00	34.22	A
ATOM	805	OG	SER	A	150	74.954	113.257	18.689	1.00	34.22	A
ATOM	806	C	SER	A	150	77.153	113.017	16.892	1.00	33.63	A

FIGURE 2 Continued

ATOM	807	O	SER	A	150	78.196	113.645	17.061	1.00	33.63	A
ATOM	808	N	ASN	A	151	76.331	113.267	15.885	1.00	44.56	A
ATOM	809	CA	ASN	A	151	76.615	114.323	14.927	1.00	44.56	A
ATOM	810	CB	ASN	A	151	76.181	113.882	13.523	1.00	38.21	A
ATOM	811	CG	ASN	A	151	76.577	114.876	12.442	1.00	38.21	A
ATOM	812	OD1	ASN	A	151	77.750	115.243	12.312	1.00	38.21	A
ATOM	813	ND2	ASN	A	151	75.602	115.306	11.650	1.00	38.21	A
ATOM	814	C	ASN	A	151	75.796	115.524	15.370	1.00	44.56	A
ATOM	815	O	ASN	A	151	75.771	116.556	14.705	1.00	44.56	A
ATOM	816	N	LEU	A	152	75.140	115.383	16.515	1.00	38.69	A
ATOM	817	CA	LEU	A	152	74.278	116.433	17.033	1.00	38.69	A
ATOM	818	CB	LEU	A	152	72.847	115.903	17.110	1.00	51.68	A
ATOM	819	CG	LEU	A	152	71.680	116.886	17.141	1.00	51.68	A
ATOM	820	CD1	LEU	A	152	71.588	117.618	15.814	1.00	51.68	A
ATOM	821	CD2	LEU	A	152	70.390	116.124	17.396	1.00	51.68	A
ATOM	822	C	LEU	A	152	74.697	116.952	18.403	1.00	38.69	A
ATOM	823	O	LEU	A	152	74.609	118.142	18.664	1.00	38.69	A
ATOM	824	N	TYR	A	153	75.155	116.062	19.272	1.00	47.26	A
ATOM	825	CA	TYR	A	153	75.538	116.460	20.615	1.00	47.26	A
ATOM	826	CB	TYR	A	153	74.732	115.653	21.626	1.00	46.55	A
ATOM	827	CG	TYR	A	153	73.250	115.726	21.362	1.00	46.55	A
ATOM	828	CD1	TYR	A	153	72.601	116.965	21.276	1.00	46.55	A
ATOM	829	CE1	TYR	A	153	71.237	117.047	21.012	1.00	46.55	A
ATOM	830	CD2	TYR	A	153	72.491	114.566	21.178	1.00	46.55	A
ATOM	831	CE2	TYR	A	153	71.124	114.636	20.915	1.00	46.55	A
ATOM	832	CZ	TYR	A	153	70.505	115.882	20.834	1.00	46.55	A
ATOM	833	OH	TYR	A	153	69.157	115.971	20.582	1.00	46.55	A
ATOM	834	C	TYR	A	153	77.020	116.289	20.880	1.00	47.26	A
ATOM	835	O	TYR	A	153	77.664	115.421	20.298	1.00	47.26	A
ATOM	836	N	LYS	A	154	77.548	117.118	21.773	1.00	39.81	A
ATOM	837	CA	LYS	A	154	78.962	117.092	22.133	1.00	39.81	A
ATOM	838	CB	LYS	A	154	79.797	117.695	21.014	1.00	41.23	A
ATOM	839	CG	LYS	A	154	79.470	119.159	20.787	1.00	41.23	A
ATOM	840	CD	LYS	A	154	80.408	119.822	19.798	1.00	41.23	A
ATOM	841	CE	LYS	A	154	79.997	121.272	19.545	1.00	41.23	A
ATOM	842	NZ	LYS	A	154	80.896	121.935	18.551	1.00	41.23	A
ATOM	843	C	LYS	A	154	79.194	117.933	23.381	1.00	39.81	A
ATOM	844	O	LYS	A	154	78.296	118.629	23.845	1.00	39.81	A
ATOM	845	N	HIS	A	155	80.412	117.851	23.914	1.00	48.33	A
ATOM	846	CA	HIS	A	155	80.818	118.644	25.071	1.00	48.33	A
ATOM	847	CB	HIS	A	155	82.072	118.055	25.711	1.00	37.58	A
ATOM	848	CG	HIS	A	155	81.857	116.718	26.341	1.00	37.58	A
ATOM	849	CD2	HIS	A	155	82.163	115.470	25.912	1.00	37.58	A
ATOM	850	ND1	HIS	A	155	81.246	116.562	27.567	1.00	37.58	A
ATOM	851	CE1	HIS	A	155	81.185	115.275	27.868	1.00	37.58	A
ATOM	852	NE2	HIS	A	155	81.734	114.591	26.880	1.00	37.58	A
ATOM	853	C	HIS	A	155	81.149	119.998	24.450	1.00	48.33	A
ATOM	854	O	HIS	A	155	82.192	120.161	23.823	1.00	48.33	A
ATOM	855	N	VAL	A	156	80.257	120.964	24.616	1.00	45.48	A
ATOM	856	CA	VAL	A	156	80.445	122.275	24.019	1.00	45.48	A
ATOM	857	CB	VAL	A	156	79.139	123.099	24.128	1.00	45.55	A
ATOM	858	CG1	VAL	A	156	79.352	124.481	23.590	1.00	45.55	A
ATOM	859	CG2	VAL	A	156	78.027	122.419	23.325	1.00	45.55	A
ATOM	860	C	VAL	A	156	81.632	123.085	24.554	1.00	45.48	A
ATOM	861	O	VAL	A	156	82.168	123.940	23.846	1.00	45.48	A
ATOM	862	N	ASP	A	157	82.062	122.807	25.781	1.00	46.18	A
ATOM	863	CA	ASP	A	157	83.181	123.540	26.355	1.00	46.18	A

FIGURE 2 Continued

ATOM	864	CB	ASP	A	157	83.130	123.485	27.892	1.00	48.96	A
ATOM	865	CG	ASP	A	157	83.086	122.063	28.437	1.00	48.96	A
ATOM	866	OD1	ASP	A	157	83.180	121.101	27.642	1.00	48.96	A
ATOM	867	OD2	ASP	A	157	82.961	121.911	29.674	1.00	48.96	A
ATOM	868	C	ASP	A	157	84.548	123.069	25.856	1.00	46.18	A
ATOM	869	O	ASP	A	157	85.434	123.890	25.606	1.00	46.18	A
ATOM	870	N	THR	A	158	84.726	121.760	25.704	1.00	43.07	A
ATOM	871	CA	THR	A	158	86.001	121.235	25.235	1.00	43.07	A
ATOM	872	CB	THR	A	158	86.454	119.998	26.038	1.00	38.95	A
ATOM	873	OG1	THR	A	158	85.542	118.914	25.816	1.00	38.95	A
ATOM	874	CG2	THR	A	158	86.512	120.321	27.523	1.00	38.95	A
ATOM	875	C	THR	A	158	85.954	120.839	23.773	1.00	43.07	A
ATOM	876	O	THR	A	158	86.990	120.643	23.149	1.00	43.07	A
ATOM	877	N	GLY	A	159	84.753	120.729	23.220	1.00	46.65	A
ATOM	878	CA	GLY	A	159	84.631	120.321	21.831	1.00	46.65	A
ATOM	879	C	GLY	A	159	84.608	118.805	21.691	1.00	46.65	A
ATOM	880	O	GLY	A	159	84.226	118.280	20.649	1.00	46.65	A
ATOM	881	N	ARG	A	160	85.015	118.099	22.741	1.00	45.58	A
ATOM	882	CA	ARG	A	160	85.013	116.642	22.722	1.00	45.58	A
ATOM	883	CB	ARG	A	160	85.470	116.088	24.068	1.00	96.26	A
ATOM	884	CG	ARG	A	160	86.942	116.275	24.330	1.00	96.26	A
ATOM	885	CD	ARG	A	160	87.299	115.755	25.706	1.00	96.26	A
ATOM	886	NE	ARG	A	160	88.721	115.899	25.991	1.00	96.26	A
ATOM	887	CZ	ARG	A	160	89.679	115.244	25.345	1.00	96.26	A
ATOM	888	NH1	ARG	A	160	89.370	114.395	24.374	1.00	96.26	A
ATOM	889	NH2	ARG	A	160	90.949	115.439	25.671	1.00	96.26	A
ATOM	890	C	ARG	A	160	83.633	116.070	22.371	1.00	45.58	A
ATOM	891	O	ARG	A	160	82.584	116.611	22.758	1.00	45.58	A
ATOM	892	N	ARG	A	161	83.658	114.950	21.658	1.00	34.58	A
ATOM	893	CA	ARG	A	161	82.452	114.287	21.197	1.00	34.58	A
ATOM	894	CB	ARG	A	161	82.776	113.570	19.885	1.00	44.43	A
ATOM	895	CG	ARG	A	161	83.066	114.552	18.778	1.00	44.43	A
ATOM	896	CD	ARG	A	161	81.783	115.300	18.531	1.00	44.43	A
ATOM	897	NE	ARG	A	161	81.951	116.561	17.844	1.00	44.43	A
ATOM	898	CZ	ARG	A	161	80.971	117.170	17.186	1.00	44.43	A
ATOM	899	NH1	ARG	A	161	79.764	116.616	17.124	1.00	44.43	A
ATOM	900	NH2	ARG	A	161	81.196	118.344	16.613	1.00	44.43	A
ATOM	901	C	ARG	A	161	81.806	113.328	22.177	1.00	34.58	A
ATOM	902	O	ARG	A	161	82.406	112.957	23.182	1.00	34.58	A
ATOM	903	N	TYR	A	162	80.557	112.972	21.890	1.00	34.84	A
ATOM	904	CA	TYR	A	162	79.796	112.006	22.688	1.00	34.84	A
ATOM	905	CB	TYR	A	162	78.312	112.381	22.751	1.00	45.35	A
ATOM	906	CG	TYR	A	162	77.922	113.462	23.741	1.00	45.35	A
ATOM	907	CD1	TYR	A	162	78.879	114.179	24.462	1.00	45.35	A
ATOM	908	CE1	TYR	A	162	78.500	115.160	25.369	1.00	45.35	A
ATOM	909	CD2	TYR	A	162	76.578	113.760	23.952	1.00	45.35	A
ATOM	910	CE2	TYR	A	162	76.188	114.730	24.843	1.00	45.35	A
ATOM	911	CZ	TYR	A	162	77.140	115.432	25.556	1.00	45.35	A
ATOM	912	OH	TYR	A	162	76.717	116.395	26.452	1.00	45.35	A
ATOM	913	C	TYR	A	162	79.927	110.696	21.909	1.00	34.84	A
ATOM	914	O	TYR	A	162	79.444	110.594	20.776	1.00	34.84	A
ATOM	915	N	TYR	A	163	80.567	109.696	22.502	1.00	38.71	A
ATOM	916	CA	TYR	A	163	80.762	108.434	21.804	1.00	38.71	A
ATOM	917	CB	TYR	A	163	82.221	107.976	21.935	1.00	34.22	A
ATOM	918	CG	TYR	A	163	83.200	108.867	21.218	1.00	34.22	A
ATOM	919	CD1	TYR	A	163	83.679	110.035	21.815	1.00	34.22	A
ATOM	920	CE1	TYR	A	163	84.518	110.905	21.123	1.00	34.22	A

FIGURE 2 Continued

ATOM	921	CD2	TYR	A	163	83.591	108.585	19.908	1.00	34.22	A
ATOM	922	CE2	TYR	A	163	84.421	109.445	19.205	1.00	34.22	A
ATOM	923	CZ	TYR	A	163	84.881	110.607	19.818	1.00	34.22	A
ATOM	924	OH	TYR	A	163	85.677	111.471	19.111	1.00	34.22	A
ATOM	925	C	TYR	A	163	79.870	107.278	22.210	1.00	38.71	A
ATOM	926	O	TYR	A	163	79.588	107.073	23.397	1.00	38.71	A
ATOM	927	N	VAL	A	164	79.429	106.522	21.203	1.00	30.31	A
ATOM	928	CA	VAL	A	164	78.633	105.321	21.434	1.00	30.31	A
ATOM	929	CB	VAL	A	164	78.267	104.608	20.108	1.00	28.31	A
ATOM	930	CG1	VAL	A	164	77.683	103.227	20.409	1.00	28.31	A
ATOM	931	CG2	VAL	A	164	77.282	105.458	19.290	1.00	28.31	A
ATOM	932	C	VAL	A	164	79.600	104.419	22.199	1.00	30.31	A
ATOM	933	O	VAL	A	164	80.785	104.361	21.859	1.00	30.31	A
ATOM	934	N	ALA	A	165	79.119	103.714	23.219	1.00	32.57	A
ATOM	935	CA	ALA	A	165	80.015	102.860	23.975	1.00	32.57	A
ATOM	936	CB	ALA	A	165	80.900	103.714	24.875	1.00	45.92	A
ATOM	937	C	ALA	A	165	79.332	101.792	24.804	1.00	32.57	A
ATOM	938	O	ALA	A	165	78.219	101.982	25.296	1.00	32.57	A
ATOM	939	N	LEU	A	166	80.012	100.660	24.953	1.00	42.13	A
ATOM	940	CA	LEU	A	166	79.498	99.565	25.756	1.00	42.13	A
ATOM	941	CB	LEU	A	166	79.302	98.305	24.906	1.00	36.18	A
ATOM	942	CG	LEU	A	166	78.240	98.396	23.805	1.00	36.18	A
ATOM	943	CD1	LEU	A	166	78.150	97.066	23.063	1.00	36.18	A
ATOM	944	CD2	LEU	A	166	76.897	98.760	24.412	1.00	36.18	A
ATOM	945	C	LEU	A	166	80.530	99.311	26.847	1.00	42.13	A
ATOM	946	O	LEU	A	166	81.726	99.233	26.571	1.00	42.13	A
ATOM	947	N	ASN	A	167	80.067	99.190	28.086	1.00	44.32	A
ATOM	948	CA	ASN	A	167	80.965	98.960	29.206	1.00	44.32	A
ATOM	949	CB	ASN	A	167	80.219	99.214	30.509	1.00	45.55	A
ATOM	950	CG	ASN	A	167	79.882	100.672	30.692	1.00	45.55	A
ATOM	951	OD1	ASN	A	167	80.775	101.516	30.692	1.00	45.55	A
ATOM	952	ND2	ASN	A	167	78.595	100.983	30.837	1.00	45.55	A
ATOM	953	C	ASN	A	167	81.605	97.575	29.232	1.00	44.32	A
ATOM	954	O	ASN	A	167	81.255	96.699	28.432	1.00	44.32	A
ATOM	955	N	LYS	A	168	82.556	97.387	30.149	1.00	50.03	A
ATOM	956	CA	LYS	A	168	83.242	96.106	30.287	1.00	50.03	A
ATOM	957	CB	LYS	A	168	84.227	96.132	31.457	1.00	71.50	A
ATOM	958	CG	LYS	A	168	85.484	96.916	31.193	1.00	71.50	A
ATOM	959	CD	LYS	A	168	86.451	96.793	32.362	1.00	71.50	A
ATOM	960	CE	LYS	A	168	87.746	97.558	32.103	1.00	71.50	A
ATOM	961	NZ	LYS	A	168	88.618	97.592	33.318	1.00	71.50	A
ATOM	962	C	LYS	A	168	82.245	94.986	30.513	1.00	50.03	A
ATOM	963	O	LYS	A	168	82.538	93.832	30.235	1.00	50.03	A
ATOM	964	N	ASP	A	169	81.066	95.337	31.013	1.00	53.99	A
ATOM	965	CA	ASP	A	169	80.020	94.360	31.291	1.00	53.99	A
ATOM	966	CB	ASP	A	169	79.415	94.635	32.668	1.00	59.01	A
ATOM	967	CG	ASP	A	169	78.633	95.939	32.714	1.00	59.01	A
ATOM	968	OD1	ASP	A	169	78.901	96.840	31.889	1.00	59.01	A
ATOM	969	OD2	ASP	A	169	77.751	96.068	33.589	1.00	59.01	A
ATOM	970	C	ASP	A	169	78.914	94.354	30.234	1.00	53.99	A
ATOM	971	O	ASP	A	169	77.797	93.903	30.503	1.00	53.99	A
ATOM	972	N	GLY	A	170	79.220	94.865	29.040	1.00	48.11	A
ATOM	973	CA	GLY	A	170	78.243	94.876	27.960	1.00	48.11	A
ATOM	974	C	GLY	A	170	77.100	95.855	28.136	1.00	48.11	A
ATOM	975	O	GLY	A	170	76.172	95.902	27.331	1.00	48.11	A
ATOM	976	N	THR	A	171	77.161	96.629	29.207	1.00	39.40	A
ATOM	977	CA	THR	A	171	76.148	97.637	29.493	1.00	39.40	A

FIGURE 2 Continued

ATOM	978	CB	THR	A	171	76.218	98.067	30.972	1.00	60.37	A
ATOM	979	OG1	THR	A	171	75.692	97.024	31.794	1.00	60.37	A
ATOM	980	CG2	THR	A	171	75.418	99.327	31.207	1.00	60.37	A
ATOM	981	C	THR	A	171	76.371	98.876	28.615	1.00	39.40	A
ATOM	982	O	THR	A	171	77.514	99.259	28.339	1.00	39.40	A
ATOM	983	N	PRO	A	172	75.284	99.497	28.132	1.00	35.13	A
ATOM	984	CD	PRO	A	172	73.846	99.191	28.235	1.00	29.81	A
ATOM	985	CA	PRO	A	172	75.519	100.686	27.312	1.00	35.13	A
ATOM	986	CB	PRO	A	172	74.136	100.988	26.732	1.00	29.81	A
ATOM	987	CG	PRO	A	172	73.209	100.500	27.800	1.00	29.81	A
ATOM	988	C	PRO	A	172	76.040	101.792	28.243	1.00	35.13	A
ATOM	989	O	PRO	A	172	75.635	101.875	29.401	1.00	35.13	A
ATOM	990	N	ARG	A	173	76.958	102.615	27.752	1.00	41.92	A
ATOM	991	CA	ARG	A	173	77.502	103.681	28.567	1.00	41.92	A
ATOM	992	CB	ARG	A	173	79.034	103.692	28.475	1.00	50.58	A
ATOM	993	CG	ARG	A	173	79.684	104.942	29.049	1.00	50.58	A
ATOM	994	CD	ARG	A	173	81.198	104.844	29.090	1.00	50.58	A
ATOM	995	NE	ARG	A	173	81.650	104.278	30.353	1.00	50.58	A
ATOM	996	CZ	ARG	A	173	82.123	104.986	31.378	1.00	50.58	A
ATOM	997	NH1	ARG	A	173	82.224	106.304	31.296	1.00	50.58	A
ATOM	998	NH2	ARG	A	173	82.465	104.372	32.504	1.00	50.58	A
ATOM	999	C	ARG	A	173	76.935	105.029	28.142	1.00	41.92	A
ATOM	1000	O	ARG	A	173	76.502	105.208	27.000	1.00	41.92	A
ATOM	1001	N	GLU	A	174	76.913	105.974	29.074	1.00	35.06	A
ATOM	1002	CA	GLU	A	174	76.427	107.310	28.771	1.00	35.06	A
ATOM	1003	CB	GLU	A	174	76.381	108.174	30.041	1.00	68.78	A
ATOM	1004	CG	GLU	A	174	75.527	107.601	31.165	1.00	68.78	A
ATOM	1005	CD	GLU	A	174	76.269	106.590	32.042	1.00	68.78	A
ATOM	1006	OE1	GLU	A	174	77.015	105.741	31.506	1.00	68.78	A
ATOM	1007	OE2	GLU	A	174	76.092	106.635	33.280	1.00	68.78	A
ATOM	1008	C	GLU	A	174	77.429	107.885	27.779	1.00	35.06	A
ATOM	1009	O	GLU	A	174	78.635	107.877	28.036	1.00	35.06	A
ATOM	1010	N	GLY	A	175	76.936	108.372	26.647	1.00	35.16	A
ATOM	1011	CA	GLY	A	175	77.825	108.928	25.638	1.00	35.16	A
ATOM	1012	C	GLY	A	175	78.479	110.182	26.152	1.00	35.16	A
ATOM	1013	O	GLY	A	175	79.390	110.750	25.554	1.00	35.16	A
ATOM	1014	N	THR	A	176	77.996	110.597	27.304	1.00	46.74	A
ATOM	1015	CA	THR	A	176	78.455	111.786	27.970	1.00	46.74	A
ATOM	1016	CB	THR	A	176	77.329	112.261	28.905	1.00	43.51	A
ATOM	1017	OG1	THR	A	176	77.021	113.627	28.612	1.00	43.51	A
ATOM	1018	CG2	THR	A	176	77.704	112.079	30.356	1.00	43.51	A
ATOM	1019	C	THR	A	176	79.753	111.539	28.743	1.00	46.74	A
ATOM	1020	O	THR	A	176	80.500	112.472	29.042	1.00	46.74	A
ATOM	1021	N	ARG	A	177	80.021	110.275	29.057	1.00	35.63	A
ATOM	1022	CA	ARG	A	177	81.209	109.906	29.815	1.00	35.63	A
ATOM	1023	CB	ARG	A	177	80.809	109.139	31.078	1.00	62.21	A
ATOM	1024	CG	ARG	A	177	79.688	109.778	31.882	1.00	62.21	A
ATOM	1025	CD	ARG	A	177	79.780	109.366	33.335	1.00	62.21	A
ATOM	1026	NE	ARG	A	177	79.794	107.916	33.496	1.00	62.21	A
ATOM	1027	CZ	ARG	A	177	80.449	107.278	34.464	1.00	62.21	A
ATOM	1028	NH1	ARG	A	177	81.146	107.973	35.353	1.00	62.21	A
ATOM	1029	NH2	ARG	A	177	80.418	105.952	34.544	1.00	62.21	A
ATOM	1030	C	ARG	A	177	82.143	109.046	28.973	1.00	35.63	A
ATOM	1031	O	ARG	A	177	82.503	107.936	29.366	1.00	35.63	A
ATOM	1032	N	THR	A	178	82.546	109.561	27.817	1.00	30.90	A
ATOM	1033	CA	THR	A	178	83.418	108.798	26.940	1.00	30.90	A
ATOM	1034	CB	THR	A	178	82.591	108.089	25.827	1.00	28.20	A

FIGURE 2 Continued

ATOM	1035	OG1	THR	A	178	81.824	109.064	25.103	1.00	28.20	A
ATOM	1036	CG2	THR	A	178	81.647	107.050	26.428	1.00	28.20	A
ATOM	1037	C	THR	A	178	84.460	109.684	26.280	1.00	30.90	A
ATOM	1038	O	THR	A	178	84.258	110.885	26.146	1.00	30.90	A
ATOM	1039	N	LYS	A	179	85.576	109.081	25.876	1.00	48.41	A
ATOM	1040	CA	LYS	A	179	86.653	109.796	25.192	1.00	48.41	A
ATOM	1041	CB	LYS	A	179	87.788	110.138	26.161	1.00	69.90	A
ATOM	1042	CG	LYS	A	179	87.432	111.284	27.091	1.00	69.90	A
ATOM	1043	CD	LYS	A	179	88.603	111.775	27.929	1.00	69.90	A
ATOM	1044	CE	LYS	A	179	88.180	112.976	28.798	1.00	69.90	A
ATOM	1045	NZ	LYS	A	179	89.250	113.510	29.718	1.00	69.90	A
ATOM	1046	C	LYS	A	179	87.154	108.920	24.049	1.00	48.41	A
ATOM	1047	O	LYS	A	179	87.414	107.733	24.235	1.00	48.41	A
ATOM	1048	N	ARG	A	180	87.264	109.521	22.867	1.00	46.56	A
ATOM	1049	CA	ARG	A	180	87.685	108.842	21.645	1.00	46.56	A
ATOM	1050	CB	ARG	A	180	88.307	109.849	20.667	1.00	34.05	A
ATOM	1051	CG	ARG	A	180	88.731	109.224	19.338	1.00	34.05	A
ATOM	1052	CD	ARG	A	180	89.535	110.180	18.467	1.00	34.05	A
ATOM	1053	NE	ARG	A	180	88.754	111.329	18.014	1.00	34.05	A
ATOM	1054	CZ	ARG	A	180	87.997	111.348	16.920	1.00	34.05	A
ATOM	1055	NH1	ARG	A	180	87.906	110.278	16.140	1.00	34.05	A
ATOM	1056	NH2	ARG	A	180	87.322	112.446	16.606	1.00	34.05	A
ATOM	1057	C	ARG	A	180	88.632	107.652	21.774	1.00	46.56	A
ATOM	1058	O	ARG	A	180	88.379	106.595	21.200	1.00	46.56	A
ATOM	1059	N	HIS	A	181	89.716	107.807	22.523	1.00	45.11	A
ATOM	1060	CA	HIS	A	181	90.692	106.728	22.636	1.00	45.11	A
ATOM	1061	CB	HIS	A	181	92.085	107.309	22.885	1.00	51.67	A
ATOM	1062	CG	HIS	A	181	92.527	108.261	21.820	1.00	51.67	A
ATOM	1063	CD2	HIS	A	181	93.044	109.510	21.897	1.00	51.67	A
ATOM	1064	ND1	HIS	A	181	92.419	107.970	20.476	1.00	51.67	A
ATOM	1065	CE1	HIS	A	181	92.848	109.001	19.770	1.00	51.67	A
ATOM	1066	NE2	HIS	A	181	93.232	109.949	20.607	1.00	51.67	A
ATOM	1067	C	HIS	A	181	90.410	105.633	23.638	1.00	45.11	A
ATOM	1068	O	HIS	A	181	91.122	104.637	23.675	1.00	45.11	A
ATOM	1069	N	GLN	A	182	89.386	105.800	24.458	1.00	45.11	A
ATOM	1070	CA	GLN	A	182	89.058	104.758	25.420	1.00	45.11	A
ATOM	1071	CB	GLN	A	182	87.965	105.241	26.375	1.00	50.78	A
ATOM	1072	CG	GLN	A	182	88.422	106.365	27.291	1.00	50.78	A
ATOM	1073	CD	GLN	A	182	87.339	106.820	28.247	1.00	50.78	A
ATOM	1074	OE1	GLN	A	182	86.362	107.459	27.848	1.00	50.78	A
ATOM	1075	NE2	GLN	A	182	87.501	106.481	29.520	1.00	50.78	A
ATOM	1076	C	GLN	A	182	88.595	103.508	24.661	1.00	45.11	A
ATOM	1077	O	GLN	A	182	87.964	103.597	23.601	1.00	45.11	A
ATOM	1078	N	LYS	A	183	88.916	102.342	25.204	1.00	45.48	A
ATOM	1079	CA	LYS	A	183	88.547	101.092	24.565	1.00	45.48	A
ATOM	1080	CB	LYS	A	183	89.126	99.911	25.354	1.00	99.67	A
ATOM	1081	CG	LYS	A	183	90.302	99.222	24.663	1.00	99.67	A
ATOM	1082	CD	LYS	A	183	91.509	100.142	24.485	1.00	99.67	A
ATOM	1083	CE	LYS	A	183	92.404	99.664	23.338	1.00	99.67	A
ATOM	1084	NZ	LYS	A	183	92.761	98.212	23.414	1.00	99.67	A
ATOM	1085	C	LYS	A	183	87.049	100.886	24.345	1.00	45.48	A
ATOM	1086	O	LYS	A	183	86.654	100.395	23.290	1.00	45.48	A
ATOM	1087	N	PHE	A	184	86.214	101.281	25.308	1.00	36.90	A
ATOM	1088	CA	PHE	A	184	84.780	101.067	25.157	1.00	36.90	A
ATOM	1089	CB	PHE	A	184	84.030	101.259	26.492	1.00	45.30	A
ATOM	1090	CG	PHE	A	184	84.341	102.541	27.220	1.00	45.30	A
ATOM	1091	CD1	PHE	A	184	84.490	103.749	26.540	1.00	45.30	A

FIGURE 2 Continued

ATOM	1092	CD2	PHE	A	184	84.427	102.543	28.609	1.00	45.30	A
ATOM	1093	CE1	PHE	A	184	84.718	104.946	27.237	1.00	45.30	A
ATOM	1094	CE2	PHE	A	184	84.651	103.721	29.317	1.00	45.30	A
ATOM	1095	CZ	PHE	A	184	84.798	104.930	28.629	1.00	45.30	A
ATOM	1096	C	PHE	A	184	84.083	101.849	24.049	1.00	36.90	A
ATOM	1097	O	PHE	A	184	82.867	101.707	23.854	1.00	36.90	A
ATOM	1098	N	THR	A	185	84.847	102.652	23.311	1.00	33.33	A
ATOM	1099	CA	THR	A	185	84.290	103.432	22.206	1.00	33.33	A
ATOM	1100	CB	THR	A	185	84.769	104.905	22.259	1.00	42.77	A
ATOM	1101	OG1	THR	A	185	86.196	104.951	22.168	1.00	42.77	A
ATOM	1102	CG2	THR	A	185	84.343	105.556	23.556	1.00	42.77	A
ATOM	1103	C	THR	A	185	84.704	102.832	20.852	1.00	33.33	A
ATOM	1104	O	THR	A	185	84.244	103.260	19.792	1.00	33.33	A
ATOM	1105	N	HIS	A	186	85.567	101.826	20.895	1.00	33.46	A
ATOM	1106	CA	HIS	A	186	86.051	101.201	19.670	1.00	33.46	A
ATOM	1107	CB	HIS	A	186	87.455	100.639	19.900	1.00	42.98	A
ATOM	1108	CG	HIS	A	186	88.440	101.672	20.357	1.00	42.98	A
ATOM	1109	CD2	HIS	A	186	88.292	102.998	20.591	1.00	42.98	A
ATOM	1110	ND1	HIS	A	186	89.760	101.380	20.629	1.00	42.98	A
ATOM	1111	CE1	HIS	A	186	90.380	102.482	21.012	1.00	42.98	A
ATOM	1112	NE2	HIS	A	186	89.513	103.477	20.998	1.00	42.98	A
ATOM	1113	C	HIS	A	186	85.114	100.115	19.190	1.00	33.46	A
ATOM	1114	O	HIS	A	186	84.886	99.122	19.885	1.00	33.46	A
ATOM	1115	N	PHE	A	187	84.566	100.319	17.997	1.00	36.19	A
ATOM	1116	CA	PHE	A	187	83.644	99.361	17.412	1.00	36.19	A
ATOM	1117	CB	PHE	A	187	82.236	99.947	17.310	1.00	32.14	A
ATOM	1118	CG	PHE	A	187	81.518	100.047	18.619	1.00	32.14	A
ATOM	1119	CD1	PHE	A	187	81.684	101.161	19.442	1.00	32.14	A
ATOM	1120	CD2	PHE	A	187	80.640	99.037	19.024	1.00	32.14	A
ATOM	1121	CE1	PHE	A	187	80.984	101.270	20.648	1.00	32.14	A
ATOM	1122	CE2	PHE	A	187	79.936	99.140	20.234	1.00	32.14	A
ATOM	1123	CZ	PHE	A	187	80.108	100.262	21.044	1.00	32.14	A
ATOM	1124	C	PHE	A	187	84.084	98.913	16.025	1.00	36.19	A
ATOM	1125	O	PHE	A	187	84.286	99.726	15.124	1.00	36.19	A
ATOM	1126	N	LEU	A	188	84.202	97.601	15.868	1.00	35.26	A
ATOM	1127	CA	LEU	A	188	84.600	96.990	14.614	1.00	35.26	A
ATOM	1128	CB	LEU	A	188	85.540	95.821	14.911	1.00	36.91	A
ATOM	1129	CG	LEU	A	188	85.877	94.870	13.765	1.00	36.91	A
ATOM	1130	CD1	LEU	A	188	86.762	95.575	12.747	1.00	36.91	A
ATOM	1131	CD2	LEU	A	188	86.565	93.623	14.337	1.00	36.91	A
ATOM	1132	C	LEU	A	188	83.395	96.481	13.805	1.00	35.26	A
ATOM	1133	O	LEU	A	188	82.619	95.636	14.281	1.00	35.26	A
ATOM	1134	N	PRO	A	189	83.201	97.013	12.587	1.00	31.65	A
ATOM	1135	CD	PRO	A	189	83.807	98.218	11.995	1.00	16.57	A
ATOM	1136	CA	PRO	A	189	82.075	96.541	11.777	1.00	31.65	A
ATOM	1137	CB	PRO	A	189	82.037	97.526	10.605	1.00	16.57	A
ATOM	1138	CG	PRO	A	189	82.696	98.754	11.141	1.00	16.57	A
ATOM	1139	C	PRO	A	189	82.444	95.129	11.313	1.00	31.65	A
ATOM	1140	O	PRO	A	189	83.447	94.943	10.618	1.00	31.65	A
ATOM	1141	N	ARG	A	190	81.654	94.140	11.714	1.00	32.96	A
ATOM	1142	CA	ARG	A	190	81.929	92.765	11.337	1.00	32.96	A
ATOM	1143	CB	ARG	A	190	81.900	91.847	12.555	1.00	32.13	A
ATOM	1144	CG	ARG	A	190	83.004	92.081	13.543	1.00	32.13	A
ATOM	1145	CD	ARG	A	190	83.550	90.757	13.987	1.00	32.13	A
ATOM	1146	NE	ARG	A	190	82.515	89.977	14.635	1.00	32.13	A
ATOM	1147	CZ	ARG	A	190	82.240	88.701	14.375	1.00	32.13	A
ATOM	1148	NH1	ARG	A	190	82.925	88.021	13.464	1.00	32.13	A

FIGURE 2 Continued

ATOM	1149	NH2	ARG	A	190	81.264	88.106	15.044	1.00	32.13	A
ATOM	1150	C	ARG	A	190	80.914	92.288	10.332	1.00	32.96	A
ATOM	1151	O	ARG	A	190	79.806	92.812	10.258	1.00	32.96	A
ATOM	1152	N	PRO	A	191	81.277	91.274	9.540	1.00	39.93	A
ATOM	1153	CD	PRO	A	191	82.594	90.616	9.406	1.00	36.93	A
ATOM	1154	CA	PRO	A	191	80.333	90.772	8.545	1.00	39.93	A
ATOM	1155	CB	PRO	A	191	81.249	90.096	7.531	1.00	36.93	A
ATOM	1156	CG	PRO	A	191	82.321	89.520	8.405	1.00	36.93	A
ATOM	1157	C	PRO	A	191	79.306	89.816	9.133	1.00	39.93	A
ATOM	1158	O	PRO	A	191	79.425	89.352	10.269	1.00	39.93	A
ATOM	1159	N	VAL	A	192	78.282	89.542	8.343	1.00	38.04	A
ATOM	1160	CA	VAL	A	192	77.229	88.615	8.729	1.00	38.04	A
ATOM	1161	CB	VAL	A	192	75.840	89.308	8.775	1.00	40.58	A
ATOM	1162	CG1	VAL	A	192	74.745	88.259	8.965	1.00	40.58	A
ATOM	1163	CG2	VAL	A	192	75.795	90.324	9.906	1.00	40.58	A
ATOM	1164	C	VAL	A	192	77.197	87.527	7.661	1.00	38.04	A
ATOM	1165	O	VAL	A	192	77.260	87.822	6.465	1.00	38.04	A
ATOM	1166	N	ASP	A	193	77.113	86.271	8.074	1.00	39.71	A
ATOM	1167	CA	ASP	A	193	77.059	85.210	7.081	1.00	39.71	A
ATOM	1168	CB	ASP	A	193	77.427	83.865	7.695	1.00	59.08	A
ATOM	1169	CG	ASP	A	193	77.489	82.764	6.659	1.00	59.08	A
ATOM	1170	OD1	ASP	A	193	76.431	82.424	6.090	1.00	59.08	A
ATOM	1171	OD2	ASP	A	193	78.599	82.245	6.400	1.00	59.08	A
ATOM	1172	C	ASP	A	193	75.656	85.137	6.468	1.00	39.71	A
ATOM	1173	O	ASP	A	193	74.648	85.232	7.185	1.00	39.71	A
ATOM	1174	N	PRO	A	194	75.576	84.985	5.129	1.00	34.27	A
ATOM	1175	CD	PRO	A	194	76.707	84.758	4.216	1.00	39.43	A
ATOM	1176	CA	PRO	A	194	74.302	84.896	4.402	1.00	34.27	A
ATOM	1177	CB	PRO	A	194	74.742	84.621	2.966	1.00	39.43	A
ATOM	1178	CG	PRO	A	194	76.069	83.935	3.132	1.00	39.43	A
ATOM	1179	C	PRO	A	194	73.367	83.813	4.952	1.00	34.27	A
ATOM	1180	O	PRO	A	194	72.145	83.892	4.804	1.00	34.27	A
ATOM	1181	N	ASP	A	195	73.947	82.812	5.602	1.00	41.74	A
ATOM	1182	CA	ASP	A	195	73.159	81.740	6.177	1.00	41.74	A
ATOM	1183	CB	ASP	A	195	74.073	80.575	6.559	1.00	100.00	A
ATOM	1184	CG	ASP	A	195	74.763	79.963	5.340	1.00	100.00	A
ATOM	1185	OD1	ASP	A	195	74.043	79.558	4.398	1.00	100.00	A
ATOM	1186	OD2	ASP	A	195	76.015	79.893	5.313	1.00	100.00	A
ATOM	1187	C	ASP	A	195	72.381	82.269	7.376	1.00	41.74	A
ATOM	1188	O	ASP	A	195	71.441	81.630	7.846	1.00	41.74	A
ATOM	1189	N	LYS	A	196	72.767	83.451	7.851	1.00	47.47	A
ATOM	1190	CA	LYS	A	196	72.100	84.099	8.981	1.00	47.47	A
ATOM	1191	CB	LYS	A	196	73.116	84.531	10.043	1.00	52.41	A
ATOM	1192	CG	LYS	A	196	73.494	83.433	11.011	1.00	52.41	A
ATOM	1193	CD	LYS	A	196	72.315	83.101	11.900	1.00	52.41	A
ATOM	1194	CE	LYS	A	196	72.613	81.938	12.837	1.00	52.41	A
ATOM	1195	NZ	LYS	A	196	71.495	81.747	13.820	1.00	52.41	A
ATOM	1196	C	LYS	A	196	71.296	85.308	8.507	1.00	47.47	A
ATOM	1197	O	LYS	A	196	70.928	86.182	9.298	1.00	47.47	A
ATOM	1198	N	VAL	A	197	71.061	85.354	7.200	1.00	47.67	A
ATOM	1199	CA	VAL	A	197	70.259	86.397	6.564	1.00	47.67	A
ATOM	1200	CB	VAL	A	197	71.061	87.168	5.498	1.00	36.39	A
ATOM	1201	CG1	VAL	A	197	70.175	88.218	4.834	1.00	36.39	A
ATOM	1202	CG2	VAL	A	197	72.264	87.826	6.139	1.00	36.39	A
ATOM	1203	C	VAL	A	197	69.142	85.593	5.893	1.00	47.67	A
ATOM	1204	O	VAL	A	197	69.128	85.407	4.670	1.00	47.67	A
ATOM	1205	N	PRO	A	198	68.196	85.092	6.707	1.00	55.08	A

FIGURE 2 Continued

ATOM	1206	CD	PRO	A	198	68.107	85.412	8.144	1.00	48.19	A
ATOM	1207	CA	PRO	A	198	67.047	84.283	6.293	1.00	55.08	A
ATOM	1208	CB	PRO	A	198	66.324	84.004	7.614	1.00	48.19	A
ATOM	1209	CG	PRO	A	198	66.647	85.199	8.425	1.00	48.19	A
ATOM	1210	C	PRO	A	198	66.124	84.842	5.230	1.00	55.08	A
ATOM	1211	O	PRO	A	198	65.543	84.084	4.463	1.00	55.08	A
ATOM	1212	N	GLU	A	199	65.996	86.159	5.165	1.00	55.26	A
ATOM	1213	CA	GLU	A	199	65.114	86.770	4.181	1.00	55.26	A
ATOM	1214	CB	GLU	A	199	64.552	88.090	4.719	1.00	69.97	A
ATOM	1215	CG	GLU	A	199	65.592	89.187	4.918	1.00	69.97	A
ATOM	1216	CD	GLU	A	199	66.311	89.100	6.253	1.00	69.97	A
ATOM	1217	OE1	GLU	A	199	66.731	87.991	6.642	1.00	69.97	A
ATOM	1218	OE2	GLU	A	199	66.466	90.152	6.909	1.00	69.97	A
ATOM	1219	C	GLU	A	199	65.795	87.024	2.842	1.00	55.26	A
ATOM	1220	O	GLU	A	199	65.205	87.638	1.956	1.00	55.26	A
ATOM	1221	N	LEU	A	200	67.030	86.562	2.688	1.00	50.69	A
ATOM	1222	CA	LEU	A	200	67.760	86.777	1.437	1.00	50.69	A
ATOM	1223	CB	LEU	A	200	69.145	86.124	1.500	1.00	37.63	A
ATOM	1224	CG	LEU	A	200	69.911	86.143	0.174	1.00	37.63	A
ATOM	1225	CD1	LEU	A	200	70.131	87.582	-0.264	1.00	37.63	A
ATOM	1226	CD2	LEU	A	200	71.222	85.435	0.330	1.00	37.63	A
ATOM	1227	C	LEU	A	200	67.023	86.247	0.211	1.00	50.69	A
ATOM	1228	O	LEU	A	200	66.899	86.936	-0.804	1.00	50.69	A
ATOM	1229	N	TYR	A	201	66.537	85.018	0.311	1.00	43.20	A
ATOM	1230	CA	TYR	A	201	65.832	84.391	-0.794	1.00	43.20	A
ATOM	1231	CB	TYR	A	201	65.398	82.977	-0.409	1.00	40.00	A
ATOM	1232	CG	TYR	A	201	64.177	82.909	0.479	1.00	40.00	A
ATOM	1233	CD1	TYR	A	201	64.282	83.036	1.862	1.00	40.00	A
ATOM	1234	CE1	TYR	A	201	63.149	82.944	2.682	1.00	40.00	A
ATOM	1235	CD2	TYR	A	201	62.911	82.695	-0.069	1.00	40.00	A
ATOM	1236	CE2	TYR	A	201	61.782	82.604	0.735	1.00	40.00	A
ATOM	1237	CZ	TYR	A	201	61.905	82.723	2.108	1.00	40.00	A
ATOM	1238	OH	TYR	A	201	60.785	82.587	2.898	1.00	40.00	A
ATOM	1239	C	TYR	A	201	64.612	85.190	-1.239	1.00	43.20	A
ATOM	1240	O	TYR	A	201	64.202	85.112	-2.397	1.00	43.20	A
ATOM	1241	N	LYS	A	202	64.022	85.948	-0.321	1.00	49.95	A
ATOM	1242	CA	LYS	A	202	62.852	86.746	-0.666	1.00	49.95	A
ATOM	1243	CB	LYS	A	202	62.247	87.382	0.590	1.00	54.88	A
ATOM	1244	CG	LYS	A	202	61.569	86.379	1.509	1.00	54.88	A
ATOM	1245	CD	LYS	A	202	61.122	87.016	2.812	1.00	54.88	A
ATOM	1246	CE	LYS	A	202	60.494	85.975	3.731	1.00	54.88	A
ATOM	1247	NZ	LYS	A	202	60.129	86.530	5.072	1.00	54.88	A
ATOM	1248	C	LYS	A	202	63.198	87.828	-1.683	1.00	49.95	A
ATOM	1249	O	LYS	A	202	62.320	88.374	-2.341	1.00	49.95	A
ATOM	1250	N	ASP	A	203	64.485	88.115	-1.826	1.00	74.84	A
ATOM	1251	CA	ASP	A	203	64.923	89.145	-2.748	1.00	74.84	A
ATOM	1252	CB	ASP	A	203	66.152	89.851	-2.172	1.00	100.00	A
ATOM	1253	CG	ASP	A	203	65.829	90.644	-0.916	1.00	100.00	A
ATOM	1254	OD1	ASP	A	203	65.135	90.104	-0.027	1.00	100.00	A
ATOM	1255	OD2	ASP	A	203	66.272	91.805	-0.814	1.00	100.00	A
ATOM	1256	C	ASP	A	203	65.209	88.650	-4.163	1.00	74.84	A
ATOM	1257	O	ASP	A	203	65.449	89.453	-5.064	1.00	74.84	A
ATOM	1258	N	ILE	A	204	65.187	87.337	-4.371	1.00	57.37	A
ATOM	1259	CA	ILE	A	204	65.438	86.801	-5.705	1.00	57.37	A
ATOM	1260	CB	ILE	A	204	66.806	86.127	-5.819	1.00	79.68	A
ATOM	1261	CG2	ILE	A	204	67.902	87.131	-5.530	1.00	79.68	A
ATOM	1262	CG1	ILE	A	204	66.867	84.930	-4.878	1.00	79.68	A

FIGURE 2 Continued

ATOM	1263	CD1	ILE	A	204	68.091	84.086	-5.073	1.00	79.68	A
ATOM	1264	C	ILE	A	204	64.402	85.777	-6.110	1.00	57.37	A
ATOM	1265	O	ILE	A	204	64.270	85.460	-7.290	1.00	57.37	A
ATOM	1266	N	LEU	A	205	63.677	85.246	-5.133	1.00	60.17	A
ATOM	1267	CA	LEU	A	205	62.648	84.263	-5.427	1.00	60.17	A
ATOM	1268	CB	LEU	A	205	62.634	83.161	-4.365	1.00	56.15	A
ATOM	1269	CG	LEU	A	205	63.902	82.308	-4.263	1.00	56.15	A
ATOM	1270	CD1	LEU	A	205	63.609	81.088	-3.401	1.00	56.15	A
ATOM	1271	CD2	LEU	A	205	64.356	81.877	-5.647	1.00	56.15	A
ATOM	1272	C	LEU	A	205	61.288	84.938	-5.497	1.00	60.17	A
ATOM	1273	O	LEU	A	205	60.926	85.732	-4.631	1.00	60.17	A
ATOM	1274	N	SER	A	206	60.538	84.630	-6.542	1.00	52.14	A
ATOM	1275	CA	SER	A	206	59.224	85.220	-6.699	1.00	52.14	A
ATOM	1276	CB	SER	A	206	58.699	84.983	-8.111	1.00	64.56	A
ATOM	1277	OG	SER	A	206	58.375	83.620	-8.289	1.00	64.56	A
ATOM	1278	C	SER	A	206	58.304	84.547	-5.703	1.00	52.14	A
ATOM	1279	O	SER	A	206	58.417	83.347	-5.478	1.00	52.14	A
ATOM	1280	N	GLN	A	207	57.403	85.313	-5.098	1.00	49.60	A
ATOM	1281	CA	GLN	A	207	56.480	84.735	-4.140	1.00	49.60	A
ATOM	1282	CB	GLN	A	207	55.469	85.778	-3.672	1.00	67.09	A
ATOM	1283	CG	GLN	A	207	54.576	85.282	-2.555	1.00	67.09	A
ATOM	1284	CD	GLN	A	207	53.616	86.342	-2.048	1.00	67.09	A
ATOM	1285	OE1	GLN	A	207	54.011	87.481	-1.775	1.00	67.09	A
ATOM	1286	NE2	GLN	A	207	52.347	85.967	-1.902	1.00	67.09	A
ATOM	1287	C	GLN	A	207	55.776	83.624	-4.891	1.00	49.60	A
ATOM	1288	O	GLN	A	207	55.557	82.535	-4.360	1.00	49.60	A
ATOM	1289	N	SER	A	208	55.454	83.923	-6.148	1.00	75.26	A
ATOM	1290	CA	SER	A	208	54.782	83.006	-7.063	1.00	75.26	A
ATOM	1291	CB	SER	A	208	55.814	82.218	-7.864	1.00	58.83	A
ATOM	1292	OG	SER	A	208	55.178	81.248	-8.676	1.00	58.83	A
ATOM	1293	C	SER	A	208	53.811	82.041	-6.405	1.00	75.26	A
ATOM	1294	O	SER	A	208	54.081	80.825	-6.461	1.00	75.26	A
ATOM	1295	OXT	SER	A	208	52.792	82.513	-5.855	1.00	58.83	A
ATOM	1296	CB	VAL	B	51	30.891	119.792	62.005	1.00	100.00	B
ATOM	1297	CG1	VAL	B	51	30.919	120.511	63.353	1.00	100.00	B
ATOM	1298	CG2	VAL	B	51	32.285	119.318	61.613	1.00	100.00	B
ATOM	1299	C	VAL	B	51	30.374	117.548	63.085	1.00	100.00	B
ATOM	1300	O	VAL	B	51	30.018	117.621	64.265	1.00	100.00	B
ATOM	1301	N	VAL	B	51	28.515	119.051	62.370	1.00	100.00	B
ATOM	1302	CA	VAL	B	51	29.898	118.583	62.054	1.00	100.00	B
ATOM	1303	N	THR	B	52	31.164	116.577	62.628	1.00	100.00	B
ATOM	1512	CG2	ILE	B	76	42.353	94.390	71.153	1.00	81.55	B
ATOM	1513	CG1	ILE	B	76	44.350	95.309	69.924	1.00	81.55	B
ATOM	1514	CD1	ILE	B	76	45.314	94.866	70.993	1.00	81.55	B
ATOM	1515	C	ILE	B	76	42.079	92.360	68.937	1.00	71.00	B
ATOM	1516	O	ILE	B	76	41.192	92.995	68.361	1.00	71.00	B
ATOM	1517	N	PHE	B	77	41.960	91.074	69.252	1.00	91.71	B
ATOM	1518	CA	PHE	B	77	40.732	90.343	68.956	1.00	91.71	B
ATOM	1519	CB	PHE	B	77	41.006	88.848	68.783	1.00	99.97	B
ATOM	1520	CG	PHE	B	77	41.620	88.488	67.465	1.00	99.97	B
ATOM	1521	CD1	PHE	B	77	42.966	88.730	67.219	1.00	99.97	B
ATOM	1522	CD2	PHE	B	77	40.849	87.893	66.469	1.00	99.97	B
ATOM	1523	CE1	PHE	B	77	43.541	88.380	65.999	1.00	99.97	B
ATOM	1524	CE2	PHE	B	77	41.413	87.540	65.245	1.00	99.97	B
ATOM	1525	CZ	PHE	B	77	42.763	87.784	65.010	1.00	99.97	B
ATOM	1526	C	PHE	B	77	39.726	90.527	70.080	1.00	91.71	B
ATOM	1527	O	PHE	B	77	40.103	90.650	71.247	1.00	91.71	B

FIGURE 2 Continued

ATOM	1528	N	PRO	B	78	38.428	90.553	69.743	1.00	97.35	B
ATOM	1529	CD	PRO	B	78	37.844	90.388	68.401	1.00	87.91	B
ATOM	1530	CA	PRO	B	78	37.384	90.720	70.760	1.00	97.35	B
ATOM	1531	CB	PRO	B	78	36.101	90.788	69.931	1.00	87.91	B
ATOM	1532	CG	PRO	B	78	36.434	89.960	68.723	1.00	87.91	B
ATOM	1533	C	PRO	B	78	37.412	89.536	71.726	1.00	97.35	B
ATOM	1534	O	PRO	B	78	36.866	89.599	72.829	1.00	97.35	B
ATOM	1535	N	ASN	B	79	38.069	88.462	71.292	1.00	99.95	B
ATOM	1536	CA	ASN	B	79	38.216	87.257	72.098	1.00	99.95	B
ATOM	1537	CB	ASN	B	79	38.734	86.090	71.240	1.00	100.00	B
ATOM	1538	CG	ASN	B	79	37.862	85.815	70.015	1.00	100.00	B
ATOM	1539	OD1	ASN	B	79	36.646	85.635	70.135	1.00	100.00	B
ATOM	1540	ND2	ASN	B	79	38.484	85.773	68.836	1.00	100.00	B
ATOM	1541	C	ASN	B	79	39.239	87.568	73.190	1.00	99.95	B
ATOM	1542	O	ASN	B	79	39.675	86.674	73.915	1.00	99.95	B
ATOM	1543	N	GLY	B	80	39.620	88.840	73.293	1.00	89.15	B
ATOM	1544	CA	GLY	B	80	40.602	89.254	74.283	1.00	89.15	B
ATOM	1545	C	GLY	B	80	41.982	88.710	73.954	1.00	89.15	B
ATOM	1546	O	GLY	B	80	42.917	88.813	74.754	1.00	89.15	B
ATOM	1547	N	THR	B	81	42.109	88.135	72.761	1.00	99.99	B
ATOM	1548	CA	THR	B	81	43.369	87.551	72.314	1.00	99.99	B
ATOM	1549	CB	THR	B	81	43.131	86.446	71.271	1.00	78.16	B
ATOM	1550	OG1	THR	B	81	41.905	85.760	71.560	1.00	78.16	B
ATOM	1551	CG2	THR	B	81	44.288	85.454	71.292	1.00	78.16	B
ATOM	1552	C	THR	B	81	44.297	88.582	71.684	1.00	99.99	B
ATOM	1553	O	THR	B	81	43.849	89.586	71.127	1.00	99.99	B
ATOM	1554	N	ILE	B	82	45.595	88.318	71.772	1.00	86.29	B
ATOM	1555	CA	ILE	B	82	46.605	89.197	71.200	1.00	86.29	B
ATOM	1556	CB	ILE	B	82	47.455	89.883	72.299	1.00	88.37	B
ATOM	1557	CG2	ILE	B	82	48.489	90.800	71.661	1.00	88.37	B
ATOM	1558	CG1	ILE	B	82	46.551	90.676	73.249	1.00	88.37	B
ATOM	1559	CD1	ILE	B	82	45.752	91.770	72.581	1.00	88.37	B
ATOM	1560	C	ILE	B	82	47.526	88.362	70.313	1.00	86.29	B
ATOM	1561	O	ILE	B	82	47.945	87.264	70.688	1.00	86.29	B
ATOM	1562	N	GLN	B	83	47.832	88.884	69.131	1.00	100.00	B
ATOM	1563	CA	GLN	B	83	48.696	88.180	68.193	1.00	100.00	B
ATOM	1564	CB	GLN	B	83	47.939	87.010	67.565	1.00	100.00	B
ATOM	1565	CG	GLN	B	83	46.683	87.429	66.814	1.00	100.00	B
ATOM	1566	CD	GLN	B	83	45.976	86.257	66.155	1.00	100.00	B
ATOM	1567	OE1	GLN	B	83	45.524	85.330	66.831	1.00	100.00	B
ATOM	1568	NE2	GLN	B	83	45.877	86.294	64.827	1.00	100.00	B
ATOM	1569	C	GLN	B	83	49.176	89.126	67.100	1.00	100.00	B
ATOM	1570	O	GLN	B	83	49.040	90.344	67.216	1.00	100.00	B
ATOM	1571	N	GLY	B	84	49.734	88.557	66.036	1.00	100.00	B
ATOM	1572	CA	GLY	B	84	50.225	89.370	64.941	1.00	100.00	B
ATOM	1573	C	GLY	B	84	50.198	88.651	63.608	1.00	100.00	B
ATOM	1574	O	GLY	B	84	50.378	87.435	63.543	1.00	100.00	B
ATOM	1575	N	THR	B	85	49.969	89.409	62.542	1.00	100.00	B
ATOM	1576	CA	THR	B	85	49.924	88.850	61.197	1.00	100.00	B
ATOM	1577	CB	THR	B	85	48.473	88.719	60.687	1.00	91.32	B
ATOM	1578	OG1	THR	B	85	47.879	90.020	60.586	1.00	91.32	B
ATOM	1579	CG2	THR	B	85	47.653	87.862	61.635	1.00	91.32	B
ATOM	1580	C	THR	B	85	50.681	89.753	60.234	1.00	100.00	B
ATOM	1581	O	THR	B	85	50.908	90.930	60.523	1.00	100.00	B
ATOM	1582	N	ARG	B	86	51.082	89.196	59.095	1.00	97.48	B
ATOM	1583	CA	ARG	B	86	51.786	89.971	58.084	1.00	97.48	B
ATOM	1584	CB	ARG	B	86	52.687	89.066	57.238	1.00	100.00	B

FIGURE 2 Continued

ATOM	1585	CG	ARG	B	86	53.901	88.526	57.986	1.00	100.00	B
ATOM	1586	CD	ARG	B	86	54.915	87.914	57.026	1.00	100.00	B
ATOM	1587	NE	ARG	B	86	56.186	87.594	57.675	1.00	100.00	B
ATOM	1588	CZ	ARG	B	86	56.372	86.585	58.524	1.00	100.00	B
ATOM	1589	NH1	ARG	B	86	55.366	85.778	58.839	1.00	100.00	B
ATOM	1590	NH2	ARG	B	86	57.569	86.382	59.060	1.00	100.00	B
ATOM	1591	C	ARG	B	86	50.726	90.633	57.214	1.00	97.48	B
ATOM	1592	O	ARG	B	86	51.035	91.385	56.291	1.00	97.48	B
ATOM	1593	N	LYS	B	87	49.469	90.341	57.534	1.00	81.65	B
ATOM	1594	CA	LYS	B	87	48.326	90.893	56.821	1.00	81.65	B
ATOM	1595	CB	LYS	B	87	47.032	90.260	57.340	1.00	99.90	B
ATOM	1596	CG	LYS	B	87	47.053	88.734	57.419	1.00	99.90	B
ATOM	1597	CD	LYS	B	87	45.766	88.194	58.057	1.00	99.90	B
ATOM	1598	CE	LYS	B	87	45.718	86.659	58.095	1.00	99.90	B
ATOM	1599	NZ	LYS	B	87	46.750	86.049	58.985	1.00	99.90	B
ATOM	1600	C	LYS	B	87	48.280	92.405	57.051	1.00	81.65	B
ATOM	1601	O	LYS	B	87	48.296	92.864	58.194	1.00	81.65	B
ATOM	1602	N	ASP	B	88	48.235	93.173	55.967	1.00	86.01	B
ATOM	1603	CA	ASP	B	88	48.177	94.629	56.056	1.00	86.01	B
ATOM	1604	CB	ASP	B	88	48.827	95.265	54.827	1.00	72.38	B
ATOM	1605	CG	ASP	B	88	48.752	96.785	54.842	1.00	72.38	B
ATOM	1606	OD1	ASP	B	88	49.424	97.414	55.688	1.00	72.38	B
ATOM	1607	OD2	ASP	B	88	48.019	97.351	54.003	1.00	72.38	B
ATOM	1608	C	ASP	B	88	46.718	95.045	56.132	1.00	86.01	B
ATOM	1609	O	ASP	B	88	45.882	94.526	55.392	1.00	86.01	B
ATOM	1610	N	HIS	B	89	46.418	95.982	57.026	1.00	76.41	B
ATOM	1611	CA	HIS	B	89	45.055	96.468	57.215	1.00	76.41	B
ATOM	1612	CB	HIS	B	89	44.511	97.075	55.923	1.00	73.52	B
ATOM	1613	CG	HIS	B	89	44.993	98.465	55.668	1.00	73.52	B
ATOM	1614	CD2	HIS	B	89	44.362	99.658	55.768	1.00	73.52	B
ATOM	1615	ND1	HIS	B	89	46.288	98.745	55.291	1.00	73.52	B
ATOM	1616	CE1	HIS	B	89	46.434	100.052	55.170	1.00	73.52	B
ATOM	1617	NE2	HIS	B	89	45.280	100.629	55.454	1.00	73.52	B
ATOM	1618	C	HIS	B	89	44.089	95.401	57.708	1.00	76.41	B
ATOM	1619	O	HIS	B	89	42.966	95.297	57.211	1.00	76.41	B
ATOM	1620	N	SER	B	90	44.526	94.619	58.691	1.00	98.90	B
ATOM	1621	CA	SER	B	90	43.694	93.568	59.267	1.00	98.90	B
ATOM	1622	CB	SER	B	90	44.531	92.682	60.185	1.00	100.00	B
ATOM	1623	OG	SER	B	90	45.798	92.419	59.611	1.00	100.00	B
ATOM	1624	C	SER	B	90	42.581	94.220	60.080	1.00	98.90	B
ATOM	1625	O	SER	B	90	42.795	95.247	60.726	1.00	98.90	B
ATOM	1626	N	ARG	B	91	41.396	93.625	60.054	1.00	99.53	B
ATOM	1627	CA	ARG	B	91	40.263	94.167	60.797	1.00	99.53	B
ATOM	1628	CB	ARG	B	91	39.082	93.196	60.716	1.00	100.00	B
ATOM	1629	CG	ARG	B	91	38.738	92.791	59.291	1.00	100.00	B
ATOM	1630	CD	ARG	B	91	37.795	91.598	59.248	1.00	100.00	B
ATOM	1631	NE	ARG	B	91	37.910	90.876	57.982	1.00	100.00	B
ATOM	1632	CZ	ARG	B	91	39.043	90.345	57.525	1.00	100.00	B
ATOM	1633	NH1	ARG	B	91	40.166	90.453	58.225	1.00	100.00	B
ATOM	1634	NH2	ARG	B	91	39.053	89.700	56.366	1.00	100.00	B
ATOM	1635	C	ARG	B	91	40.622	94.424	62.262	1.00	99.53	B
ATOM	1636	O	ARG	B	91	40.234	95.441	62.838	1.00	99.53	B
ATOM	1637	N	PHE	B	92	41.378	93.504	62.853	1.00	81.44	B
ATOM	1638	CA	PHE	B	92	41.771	93.612	64.253	1.00	81.44	B
ATOM	1639	CB	PHE	B	92	41.654	92.238	64.912	1.00	92.47	B
ATOM	1640	CG	PHE	B	92	40.319	91.590	64.699	1.00	92.47	B
ATOM	1641	CD1	PHE	B	92	39.187	92.070	65.350	1.00	92.47	B

FIGURE 2 Continued

ATOM	1642	CD2	PHE	B	92	40.180	90.537	63.801	1.00	92.47	B
ATOM	1643	CE1	PHE	B	92	37.934	91.513	65.106	1.00	92.47	B
ATOM	1644	CE2	PHE	B	92	38.932	89.974	63.550	1.00	92.47	B
ATOM	1645	CZ	PHE	B	92	37.807	90.464	64.204	1.00	92.47	B
ATOM	1646	C	PHE	B	92	43.176	94.171	64.444	1.00	81.44	B
ATOM	1647	O	PHE	B	92	43.727	94.123	65.545	1.00	81.44	B
ATOM	1648	N	GLY	B	93	43.750	94.701	63.369	1.00	64.94	B
ATOM	1649	CA	GLY	B	93	45.084	95.276	63.441	1.00	64.94	B
ATOM	1650	C	GLY	B	93	45.008	96.790	63.383	1.00	64.94	B
ATOM	1651	O	GLY	B	93	46.012	97.488	63.533	1.00	64.94	B
ATOM	1652	N	ILE	B	94	43.799	97.292	63.153	1.00	65.52	B
ATOM	1653	CA	ILE	B	94	43.547	98.723	63.087	1.00	65.52	B
ATOM	1654	CB	ILE	B	94	42.281	99.019	62.275	1.00	52.14	B
ATOM	1655	CG2	ILE	B	94	42.051	100.520	62.197	1.00	52.14	B
ATOM	1656	CG1	ILE	B	94	42.414	98.420	60.876	1.00	52.14	B
ATOM	1657	CD1	ILE	B	94	43.591	98.947	60.092	1.00	52.14	B
ATOM	1658	C	ILE	B	94	43.346	99.202	64.518	1.00	65.52	B
ATOM	1659	O	ILE	B	94	42.261	99.070	65.082	1.00	65.52	B
ATOM	1660	N	LEU	B	95	44.408	99.750	65.096	1.00	74.57	B
ATOM	1661	CA	LEU	B	95	44.388	100.229	66.471	1.00	74.57	B
ATOM	1662	CB	LEU	B	95	45.656	99.768	67.183	1.00	54.82	B
ATOM	1663	CG	LEU	B	95	46.096	98.352	66.799	1.00	54.82	B
ATOM	1664	CD1	LEU	B	95	47.388	98.006	67.504	1.00	54.82	B
ATOM	1665	CD2	LEU	B	95	44.998	97.362	67.155	1.00	54.82	B
ATOM	1666	C	LEU	B	95	44.300	101.744	66.536	1.00	74.57	B
ATOM	1667	O	LEU	B	95	44.636	102.433	65.580	1.00	74.57	B
ATOM	1668	N	GLU	B	96	43.844	102.259	67.671	1.00	77.91	B
ATOM	1669	CA	GLU	B	96	43.727	103.697	67.860	1.00	77.91	B
ATOM	1670	CB	GLU	B	96	42.279	104.090	68.133	1.00	80.12	B
ATOM	1671	CG	GLU	B	96	42.109	105.569	68.393	1.00	80.12	B
ATOM	1672	CD	GLU	B	96	40.659	105.978	68.523	1.00	80.12	B
ATOM	1673	OE1	GLU	B	96	39.892	105.782	67.551	1.00	80.12	B
ATOM	1674	OE2	GLU	B	96	40.292	106.501	69.598	1.00	80.12	B
ATOM	1675	C	GLU	B	96	44.592	104.115	69.030	1.00	77.91	B
ATOM	1676	O	GLU	B	96	44.395	103.651	70.149	1.00	77.91	B
ATOM	1677	N	PHE	B	97	45.558	104.988	68.773	1.00	61.79	B
ATOM	1678	CA	PHE	B	97	46.438	105.440	69.832	1.00	61.79	B
ATOM	1679	CB	PHE	B	97	47.780	105.877	69.252	1.00	54.42	B
ATOM	1680	CG	PHE	B	97	48.743	104.746	69.059	1.00	54.42	B
ATOM	1681	CD1	PHE	B	97	48.385	103.631	68.307	1.00	54.42	B
ATOM	1682	CD2	PHE	B	97	50.009	104.792	69.633	1.00	54.42	B
ATOM	1683	CE1	PHE	B	97	49.274	102.570	68.129	1.00	54.42	B
ATOM	1684	CE2	PHE	B	97	50.914	103.738	69.466	1.00	54.42	B
ATOM	1685	CZ	PHE	B	97	50.546	102.624	68.710	1.00	54.42	B
ATOM	1686	C	PHE	B	97	45.831	106.552	70.672	1.00	61.79	B
ATOM	1687	O	PHE	B	97	45.244	107.503	70.154	1.00	61.79	B
ATOM	1688	N	ILE	B	98	45.976	106.402	71.983	1.00	69.37	B
ATOM	1689	CA	ILE	B	98	45.454	107.354	72.947	1.00	69.37	B
ATOM	1690	CB	ILE	B	98	44.478	106.669	73.923	1.00	53.98	B
ATOM	1691	CG2	ILE	B	98	43.824	107.704	74.821	1.00	53.98	B
ATOM	1692	CG1	ILE	B	98	43.409	105.909	73.141	1.00	53.98	B
ATOM	1693	CD1	ILE	B	98	42.536	105.039	74.009	1.00	53.98	B
ATOM	1694	C	ILE	B	98	46.607	107.913	73.760	1.00	69.37	B
ATOM	1695	O	ILE	B	98	47.311	107.164	74.438	1.00	69.37	B
ATOM	1696	N	SER	B	99	46.813	109.222	73.687	1.00	55.09	B
ATOM	1697	CA	SER	B	99	47.881	109.847	74.459	1.00	55.09	B
ATOM	1698	CB	SER	B	99	48.316	111.161	73.807	1.00	87.73	B

FIGURE 2 Continued

ATOM	1699	OG	SER	B	99	47.195	111.921	73.402	1.00	87.73	B
ATOM	1700	C	SER	B	99	47.382	110.089	75.887	1.00	55.09	B
ATOM	1701	O	SER	B	99	46.497	110.908	76.125	1.00	55.09	B
ATOM	1702	N	ILE	B	100	47.944	109.343	76.830	1.00	76.85	B
ATOM	1703	CA	ILE	B	100	47.557	109.468	78.226	1.00	76.85	B
ATOM	1704	CB	ILE	B	100	47.975	108.213	79.029	1.00	65.94	B
ATOM	1705	CG2	ILE	B	100	47.392	108.272	80.436	1.00	65.94	B
ATOM	1706	CG1	ILE	B	100	47.481	106.952	78.318	1.00	65.94	B
ATOM	1707	CD1	ILE	B	100	45.974	106.863	78.196	1.00	65.94	B
ATOM	1708	C	ILE	B	100	48.252	110.689	78.812	1.00	76.85	B
ATOM	1709	O	ILE	B	100	47.659	111.458	79.568	1.00	76.85	B
ATOM	1710	N	ALA	B	101	49.515	110.859	78.442	1.00	62.70	B
ATOM	1711	CA	ALA	B	101	50.324	111.973	78.914	1.00	62.70	B
ATOM	1712	CB	ALA	B	101	50.451	111.919	80.432	1.00	82.58	B
ATOM	1713	C	ALA	B	101	51.703	111.892	78.268	1.00	62.70	B
ATOM	1714	O	ALA	B	101	52.020	110.921	77.584	1.00	62.70	B
ATOM	1715	N	VAL	B	102	52.523	112.910	78.486	1.00	69.95	B
ATOM	1716	CA	VAL	B	102	53.856	112.924	77.909	1.00	69.95	B
ATOM	1717	CB	VAL	B	102	54.732	114.016	78.560	1.00	67.80	B
ATOM	1718	CG1	VAL	B	102	56.099	114.054	77.894	1.00	67.80	B
ATOM	1719	CG2	VAL	B	102	54.046	115.369	78.439	1.00	67.80	B
ATOM	1720	C	VAL	B	102	54.535	111.567	78.086	1.00	69.95	B
ATOM	1721	O	VAL	B	102	54.737	111.104	79.211	1.00	69.95	B
ATOM	1722	N	GLY	B	103	54.861	110.927	76.965	1.00	62.47	B
ATOM	1723	CA	GLY	B	103	55.535	109.638	77.000	1.00	62.47	B
ATOM	1724	C	GLY	B	103	54.697	108.404	77.296	1.00	62.47	B
ATOM	1725	O	GLY	B	103	55.207	107.287	77.233	1.00	62.47	B
ATOM	1726	N	LEU	B	104	53.421	108.587	77.617	1.00	62.72	B
ATOM	1727	CA	LEU	B	104	52.559	107.451	77.925	1.00	62.72	B
ATOM	1728	CB	LEU	B	104	52.017	107.569	79.355	1.00	60.54	B
ATOM	1729	CG	LEU	B	104	53.102	107.562	80.438	1.00	60.54	B
ATOM	1730	CD1	LEU	B	104	52.483	107.827	81.793	1.00	60.54	B
ATOM	1731	CD2	LEU	B	104	53.826	106.225	80.432	1.00	60.54	B
ATOM	1732	C	LEU	B	104	51.410	107.336	76.938	1.00	62.72	B
ATOM	1733	O	LEU	B	104	50.793	108.337	76.558	1.00	62.72	B
ATOM	1734	N	VAL	B	105	51.112	106.104	76.540	1.00	67.82	B
ATOM	1735	CA	VAL	B	105	50.055	105.864	75.572	1.00	67.82	B
ATOM	1736	CB	VAL	B	105	50.661	105.726	74.153	1.00	78.87	B
ATOM	1737	CG1	VAL	B	105	51.563	104.501	74.089	1.00	78.87	B
ATOM	1738	CG2	VAL	B	105	49.562	105.635	73.118	1.00	78.87	B
ATOM	1739	C	VAL	B	105	49.219	104.621	75.861	1.00	67.82	B
ATOM	1740	O	VAL	B	105	49.635	103.728	76.596	1.00	67.82	B
ATOM	1741	N	SER	B	106	48.028	104.586	75.276	1.00	62.22	B
ATOM	1742	CA	SER	B	106	47.127	103.456	75.413	1.00	62.22	B
ATOM	1743	CB	SER	B	106	45.952	103.799	76.334	1.00	66.55	B
ATOM	1744	OG	SER	B	106	46.351	103.757	77.693	1.00	66.55	B
ATOM	1745	C	SER	B	106	46.624	103.100	74.018	1.00	62.22	B
ATOM	1746	O	SER	B	106	46.182	103.969	73.267	1.00	62.22	B
ATOM	1747	N	ILE	B	107	46.699	101.820	73.676	1.00	71.03	B
ATOM	1748	CA	ILE	B	107	46.277	101.348	72.366	1.00	71.03	B
ATOM	1749	CB	ILE	B	107	47.350	100.424	71.774	1.00	50.09	B
ATOM	1750	CG2	ILE	B	107	47.005	100.075	70.333	1.00	50.09	B
ATOM	1751	CG1	ILE	B	107	48.707	101.129	71.841	1.00	50.09	B
ATOM	1752	CD1	ILE	B	107	49.880	100.225	71.627	1.00	50.09	B
ATOM	1753	C	ILE	B	107	44.951	100.606	72.455	1.00	71.03	B

FIGURE 2 Continued

ATOM	1754	O	ILE	B	107	44.796	99.703	73.268	1.00	71.03	B
ATOM	1755	N	ARG	B	108	44.000	100.990	71.612	1.00	67.11	B
ATOM	1756	CA	ARG	B	108	42.683	100.373	71.610	1.00	67.11	B
ATOM	1757	CB	ARG	B	108	41.640	101.387	72.083	1.00	90.58	B
ATOM	1758	CG	ARG	B	108	40.202	100.888	72.070	1.00	90.58	B
ATOM	1759	CD	ARG	B	108	39.249	102.023	72.410	1.00	90.58	B
ATOM	1760	NE	ARG	B	108	37.854	101.596	72.478	1.00	90.58	B
ATOM	1761	CZ	ARG	B	108	36.836	102.417	72.720	1.00	90.58	B
ATOM	1762	NH1	ARG	B	108	37.057	103.712	72.919	1.00	90.58	B
ATOM	1763	NH2	ARG	B	108	35.595	101.947	72.765	1.00	90.58	B
ATOM	1764	C	ARG	B	108	42.293	99.857	70.231	1.00	67.11	B
ATOM	1765	O	ARG	B	108	42.276	100.615	69.260	1.00	67.11	B
ATOM	1766	N	GLY	B	109	41.976	98.567	70.151	1.00	80.22	B
ATOM	1767	CA	GLY	B	109	41.570	97.988	68.884	1.00	80.22	B
ATOM	1768	C	GLY	B	109	40.281	98.641	68.423	1.00	80.22	B
ATOM	1769	O	GLY	B	109	39.260	98.554	69.097	1.00	80.22	B
ATOM	1770	N	VAL	B	110	40.326	99.308	67.278	1.00	75.17	B
ATOM	1771	CA	VAL	B	110	39.152	99.983	66.745	1.00	75.17	B
ATOM	1772	CB	VAL	B	110	39.466	100.640	65.381	1.00	54.92	B
ATOM	1773	CG1	VAL	B	110	38.246	101.380	64.858	1.00	54.92	B
ATOM	1774	CG2	VAL	B	110	40.635	101.598	65.532	1.00	54.92	B
ATOM	1775	C	VAL	B	110	37.977	99.030	66.570	1.00	75.17	B
ATOM	1776	O	VAL	B	110	36.832	99.388	66.838	1.00	75.17	B
ATOM	1777	N	ASP	B	111	38.262	97.811	66.126	1.00	88.28	B
ATOM	1778	CA	ASP	B	111	37.207	96.832	65.898	1.00	88.28	B
ATOM	1779	CB	ASP	B	111	37.692	95.765	64.915	1.00	99.99	B
ATOM	1780	CG	ASP	B	111	36.561	94.909	64.386	1.00	99.99	B
ATOM	1781	OD1	ASP	B	111	36.843	93.879	63.739	1.00	99.99	B
ATOM	1782	OD2	ASP	B	111	35.386	95.269	64.609	1.00	99.99	B
ATOM	1783	C	ASP	B	111	36.715	96.160	67.178	1.00	88.28	B
ATOM	1784	O	ASP	B	111	35.511	96.056	67.410	1.00	88.28	B
ATOM	1785	N	SER	B	112	37.648	95.708	68.007	1.00	74.39	B
ATOM	1786	CA	SER	B	112	37.299	95.031	69.249	1.00	74.39	B
ATOM	1787	CB	SER	B	112	38.474	94.166	69.717	1.00	72.09	B
ATOM	1788	OG	SER	B	112	39.561	94.964	70.147	1.00	72.09	B
ATOM	1789	C	SER	B	112	36.897	95.983	70.372	1.00	74.39	B
ATOM	1790	O	SER	B	112	36.195	95.592	71.304	1.00	74.39	B
ATOM	1791	N	GLY	B	113	37.343	97.230	70.285	1.00	83.88	B
ATOM	1792	CA	GLY	B	113	37.022	98.198	71.317	1.00	83.88	B
ATOM	1793	C	GLY	B	113	37.777	97.893	72.599	1.00	83.88	B
ATOM	1794	O	GLY	B	113	37.534	98.510	73.633	1.00	83.88	B
ATOM	1795	N	LEU	B	114	38.703	96.942	72.523	1.00	62.45	B
ATOM	1796	CA	LEU	B	114	39.496	96.536	73.679	1.00	62.45	B
ATOM	1797	CB	LEU	B	114	39.678	95.015	73.684	1.00	79.61	B
ATOM	1798	CG	LEU	B	114	38.432	94.133	73.635	1.00	79.61	B
ATOM	1799	CD1	LEU	B	114	38.853	92.673	73.583	1.00	79.61	B
ATOM	1800	CD2	LEU	B	114	37.561	94.406	74.849	1.00	79.61	B
ATOM	1801	C	LEU	B	114	40.873	97.189	73.724	1.00	62.45	B
ATOM	1802	O	LEU	B	114	41.572	97.274	72.714	1.00	62.45	B
ATOM	1803	N	TYR	B	115	41.268	97.633	74.908	1.00	69.80	B
ATOM	1804	CA	TYR	B	115	42.563	98.265	75.078	1.00	69.80	B
ATOM	1805	CB	TYR	B	115	42.538	99.217	76.283	1.00	74.19	B
ATOM	1806	CG	TYR	B	115	41.461	100.277	76.176	1.00	74.19	B
ATOM	1807	CD1	TYR	B	115	40.118	99.958	76.388	1.00	74.19	B
ATOM	1808	CE1	TYR	B	115	39.114	100.904	76.205	1.00	74.19	B
ATOM	1809	CD2	TYR	B	115	41.771	101.578	75.784	1.00	74.19	B
ATOM	1810	CE2	TYR	B	115	40.772	102.530	75.597	1.00	74.19	B

FIGURE 2 Continued

ATOM	1811	CZ	TYR	B	115	39.448	102.183	75.806	1.00	74.19	B
ATOM	1812	OH	TYR	B	115	38.455	103.106	75.589	1.00	74.19	B
ATOM	1813	C	TYR	B	115	43.616	97.189	75.280	1.00	69.80	B
ATOM	1814	O	TYR	B	115	43.314	96.100	75.759	1.00	69.80	B
ATOM	1815	N	LEU	B	116	44.849	97.490	74.894	1.00	74.58	B
ATOM	1816	CA	LEU	B	116	45.941	96.549	75.055	1.00	74.58	B
ATOM	1817	CB	LEU	B	116	47.096	96.895	74.114	1.00	60.23	B
ATOM	1818	CG	LEU	B	116	48.362	96.057	74.344	1.00	60.23	B
ATOM	1819	CD1	LEU	B	116	48.085	94.607	73.967	1.00	60.23	B
ATOM	1820	CD2	LEU	B	116	49.520	96.605	73.529	1.00	60.23	B
ATOM	1821	C	LEU	B	116	46.431	96.609	76.493	1.00	74.58	B
ATOM	1822	O	LEU	B	116	46.829	97.672	76.978	1.00	74.58	B
ATOM	1823	N	GLY	B	117	46.403	95.465	77.170	1.00	91.27	B
ATOM	1824	CA	GLY	B	117	46.854	95.410	78.547	1.00	91.27	B
ATOM	1825	C	GLY	B	117	47.935	94.371	78.767	1.00	91.27	B
ATOM	1826	O	GLY	B	117	48.195	93.531	77.905	1.00	91.27	B
ATOM	1827	N	MET	B	118	48.575	94.439	79.927	1.00	96.23	B
ATOM	1828	CA	MET	B	118	49.622	93.496	80.287	1.00	96.23	B
ATOM	1829	CB	MET	B	118	50.998	94.064	79.943	1.00	79.11	B
ATOM	1830	CG	MET	B	118	52.127	93.097	80.231	1.00	79.11	B
ATOM	1831	SD	MET	B	118	53.724	93.895	80.434	1.00	79.11	B
ATOM	1832	CE	MET	B	118	54.334	93.863	78.735	1.00	79.11	B
ATOM	1833	C	MET	B	118	49.536	93.238	81.789	1.00	96.23	B
ATOM	1834	O	MET	B	118	49.933	94.087	82.593	1.00	96.23	B
ATOM	1835	N	ASN	B	119	49.020	92.069	82.166	1.00	100.00	B
ATOM	1836	CA	ASN	B	119	48.871	91.724	83.578	1.00	100.00	B
ATOM	1837	CB	ASN	B	119	48.084	90.418	83.743	1.00	95.42	B
ATOM	1838	CG	ASN	B	119	48.746	89.248	83.056	1.00	95.42	B
ATOM	1839	OD1	ASN	B	119	49.948	89.022	83.207	1.00	95.42	B
ATOM	1840	ND2	ASN	B	119	47.961	88.485	82.303	1.00	95.42	B
ATOM	1841	C	ASN	B	119	50.189	91.617	84.327	1.00	100.00	B
ATOM	1842	O	ASN	B	119	51.267	91.695	83.738	1.00	100.00	B
ATOM	1843	N	GLU	B	120	50.082	91.430	85.638	1.00	93.68	B
ATOM	1844	CA	GLU	B	120	51.241	91.327	86.513	1.00	93.68	B
ATOM	1845	CB	GLU	B	120	50.785	90.913	87.908	1.00	100.00	B
ATOM	1846	CG	GLU	B	120	51.885	90.917	88.944	1.00	100.00	B
ATOM	1847	CD	GLU	B	120	51.349	90.708	90.343	1.00	100.00	B
ATOM	1848	OE1	GLU	B	120	50.724	89.652	90.590	1.00	100.00	B
ATOM	1849	OE2	GLU	B	120	51.550	91.603	91.191	1.00	100.00	B
ATOM	1850	C	GLU	B	120	52.309	90.362	86.008	1.00	93.68	B
ATOM	1851	O	GLU	B	120	53.506	90.599	86.189	1.00	93.68	B
ATOM	1852	N	LYS	B	121	51.876	89.275	85.380	1.00	100.00	B
ATOM	1853	CA	LYS	B	121	52.806	88.282	84.856	1.00	100.00	B
ATOM	1854	CB	LYS	B	121	52.047	87.025	84.416	1.00	100.00	B
ATOM	1855	CG	LYS	B	121	51.533	86.181	85.575	1.00	100.00	B
ATOM	1856	CD	LYS	B	121	50.645	85.033	85.107	1.00	100.00	B
ATOM	1857	CE	LYS	B	121	49.336	85.540	84.516	1.00	100.00	B
ATOM	1858	NZ	LYS	B	121	48.381	84.433	84.229	1.00	100.00	B
ATOM	1859	C	LYS	B	121	53.616	88.833	83.688	1.00	100.00	B
ATOM	1860	O	LYS	B	121	54.817	88.578	83.576	1.00	100.00	B
ATOM	1861	N	GLY	B	122	52.956	89.601	82.827	1.00	83.99	B
ATOM	1862	CA	GLY	B	122	53.627	90.162	81.669	1.00	83.99	B
ATOM	1863	C	GLY	B	122	52.930	89.647	80.429	1.00	83.99	B
ATOM	1864	O	GLY	B	122	53.497	89.613	79.336	1.00	83.99	B
ATOM	1865	N	GLU	B	123	51.682	89.237	80.617	1.00	89.80	B
ATOM	1866	CA	GLU	B	123	50.872	88.710	79.533	1.00	89.80	B
ATOM	1867	CB	GLU	B	123	49.971	87.587	80.046	1.00	100.00	B

FIGURE 2 Continued

ATOM	1868	CG	GLU	B	123	50.718	86.411	80.647	1.00	100.00	B
ATOM	1869	CD	GLU	B	123	49.780	85.312	81.107	1.00	100.00	B
ATOM	1870	OE1	GLU	B	123	50.277	84.266	81.576	1.00	100.00	B
ATOM	1871	OE2	GLU	B	123	48.546	85.496	81.001	1.00	100.00	B
ATOM	1872	C	GLU	B	123	50.013	89.806	78.924	1.00	89.80	B
ATOM	1873	O	GLU	B	123	49.378	90.585	79.637	1.00	89.80	B
ATOM	1874	N	LEU	B	124	49.994	89.852	77.597	1.00	86.82	B
ATOM	1875	CA	LEU	B	124	49.215	90.846	76.876	1.00	86.82	B
ATOM	1876	CB	LEU	B	124	49.876	91.146	75.524	1.00	95.45	B
ATOM	1877	CG	LEU	B	124	51.380	91.450	75.560	1.00	95.45	B
ATOM	1878	CD1	LEU	B	124	51.905	91.625	74.145	1.00	95.45	B
ATOM	1879	CD2	LEU	B	124	51.639	92.695	76.386	1.00	95.45	B
ATOM	1880	C	LEU	B	124	47.793	90.332	76.666	1.00	86.82	B
ATOM	1881	O	LEU	B	124	47.588	89.187	76.261	1.00	86.82	B
ATOM	1882	N	TYR	B	125	46.815	91.183	76.955	1.00	71.65	B
ATOM	1883	CA	TYR	B	125	45.411	90.823	76.796	1.00	71.65	B
ATOM	1884	CB	TYR	B	125	44.843	90.282	78.109	1.00	65.11	B
ATOM	1885	CG	TYR	B	125	44.833	91.299	79.235	1.00	65.11	B
ATOM	1886	CD1	TYR	B	125	45.994	91.581	79.962	1.00	65.11	B
ATOM	1887	CE1	TYR	B	125	45.991	92.540	80.980	1.00	65.11	B
ATOM	1888	CD2	TYR	B	125	43.667	92.002	79.553	1.00	65.11	B
ATOM	1889	CE2	TYR	B	125	43.653	92.959	80.564	1.00	65.11	B
ATOM	1890	CZ	TYR	B	125	44.817	93.226	81.274	1.00	65.11	B
ATOM	1891	OH	TYR	B	125	44.804	94.184	82.269	1.00	65.11	B
ATOM	1892	C	TYR	B	125	44.614	92.050	76.377	1.00	71.65	B
ATOM	1893	O	TYR	B	125	45.065	93.180	76.554	1.00	71.65	B
ATOM	1894	N	GLY	B	126	43.423	91.820	75.835	1.00	84.06	B
ATOM	1895	CA	GLY	B	126	42.585	92.919	75.396	1.00	84.06	B
ATOM	1896	C	GLY	B	126	41.552	93.336	76.420	1.00	84.06	B
ATOM	1897	O	GLY	B	126	40.406	92.894	76.367	1.00	84.06	B
ATOM	1898	N	SER	B	127	41.957	94.192	77.352	1.00	89.43	B
ATOM	1899	CA	SER	B	127	41.062	94.679	78.396	1.00	89.43	B
ATOM	1900	CB	SER	B	127	41.814	95.605	79.349	1.00	70.88	B
ATOM	1901	OG	SER	B	127	40.914	96.244	80.234	1.00	70.88	B
ATOM	1902	C	SER	B	127	39.873	95.426	77.812	1.00	89.43	B
ATOM	1903	O	SER	B	127	39.978	96.055	76.762	1.00	89.43	B
ATOM	1904	N	GLU	B	128	38.743	95.357	78.504	1.00	90.28	B
ATOM	1905	CA	GLU	B	128	37.529	96.030	78.061	1.00	90.28	B
ATOM	1906	CB	GLU	B	128	36.295	95.217	78.473	1.00	100.00	B
ATOM	1907	CG	GLU	B	128	36.226	94.850	79.962	1.00	100.00	B
ATOM	1908	CD	GLU	B	128	37.227	93.769	80.367	1.00	100.00	B
ATOM	1909	OE1	GLU	B	128	37.152	92.645	79.821	1.00	100.00	B
ATOM	1910	OE2	GLU	B	128	38.087	94.039	81.236	1.00	100.00	B
ATOM	1911	C	GLU	B	128	37.459	97.427	78.666	1.00	90.28	B
ATOM	1912	O	GLU	B	128	36.672	98.269	78.230	1.00	90.28	B
ATOM	1913	N	LYS	B	129	38.301	97.666	79.666	1.00	84.11	B
ATOM	1914	CA	LYS	B	129	38.346	98.950	80.355	1.00	84.11	B
ATOM	1915	CB	LYS	B	129	37.762	98.797	81.763	1.00	100.00	B
ATOM	1916	CG	LYS	B	129	38.379	97.651	82.556	1.00	100.00	B
ATOM	1917	CD	LYS	B	129	37.891	97.626	83.998	1.00	100.00	B
ATOM	1918	CE	LYS	B	129	38.603	96.543	84.800	1.00	100.00	B
ATOM	1919	NZ	LYS	B	129	38.260	96.610	86.246	1.00	100.00	B
ATOM	1920	C	LYS	B	129	39.775	99.490	80.442	1.00	84.11	B
ATOM	1921	O	LYS	B	129	40.734	98.731	80.603	1.00	84.11	B
ATOM	1922	N	LEU	B	130	39.910	100.809	80.345	1.00	74.10	B
ATOM	1923	CA	LEU	B	130	41.220	101.449	80.406	1.00	74.10	B
ATOM	1924	CB	LEU	B	130	41.137	102.875	79.845	1.00	62.37	B

FIGURE 2 Continued

ATOM	1925	CG	LEU	B	130	42.422	103.527	79.309	1.00	62.37	B
ATOM	1926	CD1	LEU	B	130	42.224	105.034	79.301	1.00	62.37	B
ATOM	1927	CD2	LEU	B	130	43.629	103.171	80.165	1.00	62.37	B
ATOM	1928	C	LEU	B	130	41.749	101.502	81.840	1.00	74.10	B
ATOM	1929	O	LEU	B	130	41.312	102.323	82.642	1.00	74.10	B
ATOM	1930	N	THR	B	131	42.705	100.636	82.153	1.00	71.38	B
ATOM	1931	CA	THR	B	131	43.285	100.598	83.492	1.00	71.38	B
ATOM	1932	CB	THR	B	131	43.106	99.211	84.125	1.00	71.14	B
ATOM	1933	OG1	THR	B	131	43.971	98.269	83.475	1.00	71.14	B
ATOM	1934	CG2	THR	B	131	41.666	98.754	83.972	1.00	71.14	B
ATOM	1935	C	THR	B	131	44.773	100.913	83.427	1.00	71.38	B
ATOM	1936	O	THR	B	131	45.328	101.060	82.339	1.00	71.38	B
ATOM	1937	N	GLN	B	132	45.415	101.019	84.587	1.00	71.46	B
ATOM	1938	CA	GLN	B	132	46.847	101.308	84.635	1.00	71.46	B
ATOM	1939	CB	GLN	B	132	47.331	101.378	86.080	1.00	99.65	B
ATOM	1940	CG	GLN	B	132	46.673	102.462	86.900	1.00	99.65	B
ATOM	1941	CD	GLN	B	132	47.210	102.513	88.312	1.00	99.65	B
ATOM	1942	OE1	GLN	B	132	48.407	102.703	88.525	1.00	99.65	B
ATOM	1943	NE2	GLN	B	132	46.327	102.342	89.287	1.00	99.65	B
ATOM	1944	C	GLN	B	132	47.596	100.197	83.913	1.00	71.46	B
ATOM	1945	O	GLN	B	132	48.718	100.381	83.432	1.00	71.46	B
ATOM	1946	N	GLU	B	133	46.953	99.039	83.840	1.00	99.82	B
ATOM	1947	CA	GLU	B	133	47.532	97.873	83.194	1.00	99.82	B
ATOM	1948	CB	GLU	B	133	46.774	96.625	83.657	1.00	99.09	B
ATOM	1949	CG	GLU	B	133	47.449	95.311	83.329	1.00	99.09	B
ATOM	1950	CD	GLU	B	133	47.139	94.236	84.353	1.00	99.09	B
ATOM	1951	OE1	GLU	B	133	47.585	94.371	85.513	1.00	99.09	B
ATOM	1952	OE2	GLU	B	133	46.449	93.257	84.002	1.00	99.09	B
ATOM	1953	C	GLU	B	133	47.471	98.012	81.675	1.00	99.82	B
ATOM	1954	O	GLU	B	133	47.779	97.073	80.943	1.00	99.82	B
ATOM	1955	N	CYS	B	134	47.093	99.198	81.209	1.00	83.03	B
ATOM	1956	CA	CYS	B	134	46.970	99.458	79.780	1.00	83.03	B
ATOM	1957	CB	CYS	B	134	45.496	99.634	79.420	1.00	84.81	B
ATOM	1958	SG	CYS	B	134	44.431	98.314	80.031	1.00	84.81	B
ATOM	1959	C	CYS	B	134	47.751	100.688	79.321	1.00	83.03	B
ATOM	1960	O	CYS	B	134	47.696	101.069	78.152	1.00	83.03	B
ATOM	1961	N	VAL	B	135	48.474	101.308	80.245	1.00	81.69	B
ATOM	1962	CA	VAL	B	135	49.262	102.492	79.929	1.00	81.69	B
ATOM	1963	CB	VAL	B	135	49.110	103.564	81.030	1.00	74.62	B
ATOM	1964	CG1	VAL	B	135	50.025	104.746	80.744	1.00	74.62	B
ATOM	1965	CG2	VAL	B	135	47.660	104.011	81.110	1.00	74.62	B
ATOM	1966	C	VAL	B	135	50.733	102.120	79.792	1.00	81.69	B
ATOM	1967	O	VAL	B	135	51.384	101.750	80.772	1.00	81.69	B
ATOM	1968	N	PHE	B	136	51.257	102.227	78.574	1.00	71.72	B
ATOM	1969	CA	PHE	B	136	52.648	101.880	78.327	1.00	71.72	B
ATOM	1970	CB	PHE	B	136	52.760	100.917	77.142	1.00	73.76	B
ATOM	1971	CG	PHE	B	136	51.818	99.757	77.213	1.00	73.76	B
ATOM	1972	CD1	PHE	B	136	50.474	99.913	76.877	1.00	73.76	B
ATOM	1973	CD2	PHE	B	136	52.269	98.505	77.622	1.00	73.76	B
ATOM	1974	CE1	PHE	B	136	49.593	98.837	76.944	1.00	73.76	B
ATOM	1975	CE2	PHE	B	136	51.394	97.421	77.694	1.00	73.76	B
ATOM	1976	CZ	PHE	B	136	50.054	97.587	77.353	1.00	73.76	B
ATOM	1977	C	PHE	B	136	53.537	103.077	78.054	1.00	71.72	B
ATOM	1978	O	PHE	B	136	53.069	104.158	77.690	1.00	71.72	B
ATOM	1979	N	ARG	B	137	54.833	102.863	78.234	1.00	76.13	B
ATOM	1980	CA	ARG	B	137	55.828	103.886	77.984	1.00	76.13	B
ATOM	1981	CB	ARG	B	137	57.055	103.664	78.865	1.00	99.50	B

FIGURE 2 Continued

ATOM	1982	CG	ARG	B	137	56.813	103.777	80.354	1.00	99.50	B
ATOM	1983	CD	ARG	B	137	58.113	103.522	81.104	1.00	99.50	B
ATOM	1984	NE	ARG	B	137	58.044	103.899	82.513	1.00	99.50	B
ATOM	1985	CZ	ARG	B	137	59.089	103.889	83.335	1.00	99.50	B
ATOM	1986	NH1	ARG	B	137	60.280	103.518	82.886	1.00	99.50	B
ATOM	1987	NH2	ARG	B	137	58.947	104.257	84.602	1.00	99.50	B
ATOM	1988	C	ARG	B	137	56.242	103.777	76.520	1.00	76.13	B
ATOM	1989	O	ARG	B	137	57.010	102.883	76.152	1.00	76.13	B
ATOM	1990	N	GLU	B	138	55.718	104.672	75.688	1.00	74.09	B
ATOM	1991	CA	GLU	B	138	56.057	104.688	74.272	1.00	74.09	B
ATOM	1992	CB	GLU	B	138	54.977	105.409	73.463	1.00	67.11	B
ATOM	1993	CG	GLU	B	138	55.318	105.569	71.977	1.00	67.11	B
ATOM	1994	CD	GLU	B	138	54.322	106.440	71.226	1.00	67.11	B
ATOM	1995	OE1	GLU	B	138	54.216	107.641	71.556	1.00	67.11	B
ATOM	1996	OE2	GLU	B	138	53.647	105.926	70.308	1.00	67.11	B
ATOM	1997	C	GLU	B	138	57.370	105.436	74.122	1.00	74.09	B
ATOM	1998	O	GLU	B	138	57.421	106.642	74.346	1.00	74.09	B
ATOM	1999	N	GLN	B	139	58.429	104.727	73.746	1.00	83.30	B
ATOM	2000	CA	GLN	B	139	59.731	105.360	73.576	1.00	83.30	B
ATOM	2001	CB	GLN	B	139	60.644	104.996	74.746	1.00	89.59	B
ATOM	2002	CG	GLN	B	139	60.327	105.773	76.003	1.00	89.59	B
ATOM	2003	CD	GLN	B	139	61.046	105.237	77.213	1.00	89.59	B
ATOM	2004	OE1	GLN	B	139	62.271	105.119	77.224	1.00	89.59	B
ATOM	2005	NE2	GLN	B	139	60.286	104.908	78.248	1.00	89.59	B
ATOM	2006	C	GLN	B	139	60.416	105.034	72.253	1.00	83.30	B
ATOM	2007	O	GLN	B	139	60.384	103.900	71.771	1.00	83.30	B
ATOM	2008	N	PHE	B	140	61.041	106.053	71.675	1.00	80.44	B
ATOM	2009	CA	PHE	B	140	61.734	105.930	70.401	1.00	80.44	B
ATOM	2010	CB	PHE	B	140	62.177	107.323	69.938	1.00	83.11	B
ATOM	2011	CG	PHE	B	140	62.947	107.322	68.652	1.00	83.11	B
ATOM	2012	CD1	PHE	B	140	62.299	107.126	67.437	1.00	83.11	B
ATOM	2013	CD2	PHE	B	140	64.328	107.502	68.656	1.00	83.11	B
ATOM	2014	CE1	PHE	B	140	63.017	107.110	66.243	1.00	83.11	B
ATOM	2015	CE2	PHE	B	140	65.054	107.486	67.470	1.00	83.11	B
ATOM	2016	CZ	PHE	B	140	64.396	107.290	66.260	1.00	83.11	B
ATOM	2017	C	PHE	B	140	62.948	105.001	70.461	1.00	80.44	B
ATOM	2018	O	PHE	B	140	63.762	105.090	71.380	1.00	80.44	B
ATOM	2019	N	GLU	B	141	63.059	104.109	69.480	1.00	81.14	B
ATOM	2020	CA	GLU	B	141	64.193	103.189	69.385	1.00	81.14	B
ATOM	2021	CB	GLU	B	141	63.721	101.759	69.115	1.00	72.53	B
ATOM	2022	CG	GLU	B	141	63.916	100.784	70.281	1.00	72.53	B
ATOM	2023	CD	GLU	B	141	65.369	100.650	70.732	1.00	72.53	B
ATOM	2024	OE1	GLU	B	141	65.877	101.559	71.427	1.00	72.53	B
ATOM	2025	OE2	GLU	B	141	66.005	99.631	70.386	1.00	72.53	B
ATOM	2026	C	GLU	B	141	65.070	103.659	68.226	1.00	81.14	B
ATOM	2027	O	GLU	B	141	66.069	104.353	68.426	1.00	81.14	B
ATOM	2028	N	GLU	B	142	64.684	103.277	67.012	1.00	71.75	B
ATOM	2029	CA	GLU	B	142	65.405	103.673	65.806	1.00	71.75	B
ATOM	2030	CB	GLU	B	142	66.612	102.751	65.569	1.00	100.00	B
ATOM	2031	CG	GLU	B	142	66.381	101.274	65.867	1.00	100.00	B
ATOM	2032	CD	GLU	B	142	65.314	100.650	64.990	1.00	100.00	B
ATOM	2033	OE1	GLU	B	142	65.443	100.718	63.748	1.00	100.00	B
ATOM	2034	OE2	GLU	B	142	64.347	100.085	65.543	1.00	100.00	B
ATOM	2035	C	GLU	B	142	64.482	103.677	64.587	1.00	71.75	B
ATOM	2036	O	GLU	B	142	63.506	102.926	64.532	1.00	71.75	B
ATOM	2037	N	ASN	B	143	64.791	104.541	63.622	1.00	62.98	B
ATOM	2038	CA	ASN	B	143	64.003	104.678	62.393	1.00	62.98	B

FIGURE 2 Continued

ATOM	2039	CB	ASN	B	143	64.396	103.591	61.392	1.00	76.05	B
ATOM	2040	CG	ASN	B	143	65.845	103.711	60.954	1.00	76.05	B
ATOM	2041	OD1	ASN	B	143	66.275	104.770	60.494	1.00	76.05	B
ATOM	2042	ND2	ASN	B	143	66.606	102.631	61.099	1.00	76.05	B
ATOM	2043	C	ASN	B	143	62.500	104.655	62.652	1.00	62.98	B
ATOM	2044	O	ASN	B	143	61.733	103.988	61.946	1.00	62.98	B
ATOM	2045	N	TRP	B	144	62.111	105.399	63.687	1.00	52.62	B
ATOM	2046	CA	TRP	B	144	60.731	105.559	64.131	1.00	52.62	B
ATOM	2047	CB	TRP	B	144	59.920	106.265	63.042	1.00	53.19	B
ATOM	2048	CG	TRP	B	144	60.536	107.595	62.776	1.00	53.19	B
ATOM	2049	CD2	TRP	B	144	60.559	108.711	63.674	1.00	53.19	B
ATOM	2050	CE2	TRP	B	144	61.430	109.677	63.122	1.00	53.19	B
ATOM	2051	CE3	TRP	B	144	59.934	108.986	64.899	1.00	53.19	B
ATOM	2052	CD1	TRP	B	144	61.361	107.925	61.735	1.00	53.19	B
ATOM	2053	NE1	TRP	B	144	61.906	109.172	61.940	1.00	53.19	B
ATOM	2054	CZ2	TRP	B	144	61.694	110.900	63.757	1.00	53.19	B
ATOM	2055	CZ3	TRP	B	144	60.200	110.203	65.531	1.00	53.19	B
ATOM	2056	CH2	TRP	B	144	61.071	111.143	64.957	1.00	53.19	B
ATOM	2057	C	TRP	B	144	60.014	104.331	64.664	1.00	52.62	B
ATOM	2058	O	TRP	B	144	58.783	104.248	64.653	1.00	52.62	B
ATOM	2059	N	TYR	B	145	60.801	103.378	65.143	1.00	62.69	B
ATOM	2060	CA	TYR	B	145	60.252	102.189	65.763	1.00	62.69	B
ATOM	2061	CB	TYR	B	145	61.138	100.973	65.509	1.00	63.90	B
ATOM	2062	CG	TYR	B	145	60.758	100.167	64.289	1.00	63.90	B
ATOM	2063	CD1	TYR	B	145	61.248	100.495	63.021	1.00	63.90	B
ATOM	2064	CE1	TYR	B	145	60.900	99.737	61.897	1.00	63.90	B
ATOM	2065	CD2	TYR	B	145	59.908	99.066	64.403	1.00	63.90	B
ATOM	2066	CE2	TYR	B	145	59.554	98.308	63.293	1.00	63.90	B
ATOM	2067	CZ	TYR	B	145	60.052	98.644	62.045	1.00	63.90	B
ATOM	2068	OH	TYR	B	145	59.703	97.877	60.957	1.00	63.90	B
ATOM	2069	C	TYR	B	145	60.285	102.535	67.246	1.00	62.69	B
ATOM	2070	O	TYR	B	145	61.300	103.030	67.739	1.00	62.69	B
ATOM	2071	N	ASN	B	146	59.183	102.307	67.954	1.00	75.32	B
ATOM	2072	CA	ASN	B	146	59.142	102.603	69.383	1.00	75.32	B
ATOM	2073	CB	ASN	B	146	57.928	103.481	69.738	1.00	54.84	B
ATOM	2074	CG	ASN	B	146	57.894	104.799	68.978	1.00	54.84	B
ATOM	2075	OD1	ASN	B	146	58.874	105.548	68.945	1.00	54.84	B
ATOM	2076	ND2	ASN	B	146	56.747	105.094	68.376	1.00	54.84	B
ATOM	2077	C	ASN	B	146	59.036	101.310	70.185	1.00	75.32	B
ATOM	2078	O	ASN	B	146	58.671	100.264	69.647	1.00	75.32	B
ATOM	2079	N	THR	B	147	59.367	101.389	71.472	1.00	70.49	B
ATOM	2080	CA	THR	B	147	59.253	100.244	72.373	1.00	70.49	B
ATOM	2081	CB	THR	B	147	60.500	100.064	73.272	1.00	68.35	B
ATOM	2082	OG1	THR	B	147	60.703	101.241	74.065	1.00	68.35	B
ATOM	2083	CG2	THR	B	147	61.726	99.809	72.433	1.00	68.35	B
ATOM	2084	C	THR	B	147	58.059	100.573	73.255	1.00	70.49	B
ATOM	2085	O	THR	B	147	57.739	101.745	73.450	1.00	70.49	B
ATOM	2086	N	TYR	B	148	57.396	99.550	73.776	1.00	78.77	B
ATOM	2087	CA	TYR	B	148	56.236	99.770	74.628	1.00	78.77	B
ATOM	2088	CB	TYR	B	148	54.957	99.432	73.858	1.00	75.53	B
ATOM	2089	CG	TYR	B	148	54.687	100.376	72.711	1.00	75.53	B
ATOM	2090	CD1	TYR	B	148	54.010	101.577	72.914	1.00	75.53	B
ATOM	2091	CE1	TYR	B	148	53.818	102.484	71.868	1.00	75.53	B
ATOM	2092	CD2	TYR	B	148	55.165	100.099	71.430	1.00	75.53	B
ATOM	2093	CE2	TYR	B	148	54.982	101.001	70.377	1.00	75.53	B
ATOM	2094	CZ	TYR	B	148	54.311	102.189	70.604	1.00	75.53	B
ATOM	2095	OH	TYR	B	148	54.144	103.085	69.572	1.00	75.53	B

FIGURE 2 Continued

ATOM	2096	C	TYR	B	148	56.325	98.937	75.898	1.00	78.77	B
ATOM	2097	O	TYR	B	148	56.066	97.735	75.884	1.00	78.77	B
ATOM	2098	N	SER	B	149	56.692	99.586	76.998	1.00	76.62	B
ATOM	2099	CA	SER	B	149	56.818	98.906	78.280	1.00	76.62	B
ATOM	2100	CB	SER	B	149	58.176	99.225	78.913	1.00	85.78	B
ATOM	2101	OG	SER	B	149	58.304	100.610	79.188	1.00	85.78	B
ATOM	2102	C	SER	B	149	55.701	99.308	79.240	1.00	76.62	B
ATOM	2103	O	SER	B	149	55.252	100.451	79.233	1.00	76.62	B
ATOM	2104	N	SER	B	150	55.254	98.356	80.055	1.00	83.08	B
ATOM	2105	CA	SER	B	150	54.204	98.607	81.037	1.00	83.08	B
ATOM	2106	CB	SER	B	150	53.905	97.326	81.827	1.00	82.51	B
ATOM	2107	OG	SER	B	150	52.820	97.497	82.725	1.00	82.51	B
ATOM	2108	C	SER	B	150	54.720	99.686	81.982	1.00	83.08	B
ATOM	2109	O	SER	B	150	55.834	99.582	82.488	1.00	83.08	B
ATOM	2110	N	ASN	B	151	53.925	100.726	82.212	1.00	93.75	B
ATOM	2111	CA	ASN	B	151	54.348	101.800	83.103	1.00	93.75	B
ATOM	2112	CB	ASN	B	151	53.595	103.093	82.787	1.00	72.85	B
ATOM	2113	CG	ASN	B	151	54.243	104.313	83.424	1.00	72.85	B
ATOM	2114	OD1	ASN	B	151	53.589	105.332	83.655	1.00	72.85	B
ATOM	2115	ND2	ASN	B	151	55.538	104.218	83.699	1.00	72.85	B
ATOM	2116	C	ASN	B	151	54.079	101.411	84.554	1.00	93.75	B
ATOM	2117	O	ASN	B	151	54.269	102.213	85.470	1.00	93.75	B
ATOM	2118	N	LEU	B	152	53.637	100.173	84.753	1.00	100.00	B
ATOM	2119	CA	LEU	B	152	53.325	99.667	86.085	1.00	100.00	B
ATOM	2120	CB	LEU	B	152	51.912	99.085	86.092	1.00	65.90	B
ATOM	2121	CG	LEU	B	152	51.418	98.477	87.404	1.00	65.90	B
ATOM	2122	CD1	LEU	B	152	51.607	99.481	88.535	1.00	65.90	B
ATOM	2123	CD2	LEU	B	152	49.952	98.090	87.265	1.00	65.90	B
ATOM	2124	C	LEU	B	152	54.313	98.604	86.561	1.00	100.00	B
ATOM	2125	O	LEU	B	152	55.144	98.852	87.439	1.00	100.00	B
ATOM	2126	N	TYR	B	153	54.213	97.420	85.971	1.00	97.40	B
ATOM	2127	CA	TYR	B	153	55.072	96.300	86.323	1.00	97.40	B
ATOM	2128	CB	TYR	B	153	54.394	95.004	85.896	1.00	68.51	B
ATOM	2129	CG	TYR	B	153	52.961	94.909	86.367	1.00	68.51	B
ATOM	2130	CD1	TYR	B	153	52.654	94.844	87.727	1.00	68.51	B
ATOM	2131	CE1	TYR	B	153	51.335	94.770	88.166	1.00	68.51	B
ATOM	2132	CD2	TYR	B	153	51.909	94.900	85.455	1.00	68.51	B
ATOM	2133	CE2	TYR	B	153	50.586	94.827	85.883	1.00	68.51	B
ATOM	2134	CZ	TYR	B	153	50.308	94.763	87.238	1.00	68.51	B
ATOM	2135	OH	TYR	B	153	49.004	94.697	87.659	1.00	68.51	B
ATOM	2136	C	TYR	B	153	56.449	96.407	85.676	1.00	97.40	B
ATOM	2137	O	TYR	B	153	56.563	96.618	84.470	1.00	97.40	B
ATOM	2138	N	LYS	B	154	57.490	96.252	86.488	1.00	92.05	B
ATOM	2139	CA	LYS	B	154	58.868	96.332	86.012	1.00	92.05	B
ATOM	2140	CB	LYS	B	154	59.527	97.614	86.529	1.00	97.83	B
ATOM	2141	CG	LYS	B	154	59.504	97.750	88.049	1.00	97.83	B
ATOM	2142	CD	LYS	B	154	60.187	99.027	88.521	1.00	97.83	B
ATOM	2143	CE	LYS	B	154	61.681	99.012	88.225	1.00	97.83	B
ATOM	2144	NZ	LYS	B	154	62.347	100.261	88.692	1.00	97.83	B
ATOM	2145	C	LYS	B	154	59.680	95.126	86.479	1.00	92.05	B
ATOM	2146	O	LYS	B	154	59.207	94.325	87.289	1.00	92.05	B
ATOM	2147	N	HIS	B	155	60.900	94.996	85.963	1.00	99.49	B
ATOM	2148	CA	HIS	B	155	61.768	93.891	86.355	1.00	99.49	B
ATOM	2149	CB	HIS	B	155	63.026	93.844	85.478	1.00	100.00	B
ATOM	2150	CG	HIS	B	155	63.051	92.695	84.513	1.00	100.00	B
ATOM	2151	CD2	HIS	B	155	63.943	91.689	84.346	1.00	100.00	B
ATOM	2152	ND1	HIS	B	155	62.065	92.491	83.569	1.00	100.00	B

FIGURE 2 Continued

ATOM	2153	CE1	HIS	B	155	62.349	91.410	82.864	1.00	100.00	B
ATOM	2154	NE2	HIS	B	155	63.483	90.905	83.315	1.00	100.00	B
ATOM	2155	C	HIS	B	155	62.155	94.065	87.817	1.00	99.49	B
ATOM	2156	O	HIS	B	155	63.017	94.881	88.158	1.00	99.49	B
ATOM	2157	N	VAL	B	156	61.491	93.289	88.668	1.00	100.00	B
ATOM	2158	CA	VAL	B	156	61.703	93.312	90.109	1.00	100.00	B
ATOM	2159	CB	VAL	B	156	61.149	92.012	90.760	1.00	100.00	B
ATOM	2160	CG1	VAL	B	156	59.632	91.963	90.610	1.00	100.00	B
ATOM	2161	CG2	VAL	B	156	61.776	90.780	90.107	1.00	100.00	B
ATOM	2162	C	VAL	B	156	63.159	93.506	90.537	1.00	100.00	B
ATOM	2163	O	VAL	B	156	63.501	94.514	91.162	1.00	100.00	B
ATOM	2164	N	ASP	B	157	64.014	92.550	90.188	1.00	100.00	B
ATOM	2165	CA	ASP	B	157	65.421	92.606	90.565	1.00	100.00	B
ATOM	2166	CB	ASP	B	157	66.048	91.213	90.427	1.00	100.00	B
ATOM	2167	CG	ASP	B	157	67.324	91.058	91.248	1.00	100.00	B
ATOM	2168	OD1	ASP	B	157	68.264	91.859	91.054	1.00	100.00	B
ATOM	2169	OD2	ASP	B	157	67.386	90.132	92.090	1.00	100.00	B
ATOM	2170	C	ASP	B	157	66.245	93.623	89.770	1.00	100.00	B
ATOM	2171	O	ASP	B	157	66.603	94.685	90.287	1.00	100.00	B
ATOM	2172	N	THR	B	158	66.541	93.288	88.515	1.00	99.85	B
ATOM	2173	CA	THR	B	158	67.345	94.142	87.636	1.00	99.85	B
ATOM	2174	CB	THR	B	158	67.363	93.595	86.179	1.00	100.00	B
ATOM	2175	OG1	THR	B	158	66.032	93.584	85.643	1.00	100.00	B
ATOM	2176	CG2	THR	B	158	67.926	92.180	86.148	1.00	100.00	B
ATOM	2177	C	THR	B	158	66.922	95.611	87.583	1.00	99.85	B
ATOM	2178	O	THR	B	158	67.757	96.510	87.708	1.00	99.85	B
ATOM	2179	N	GLY	B	159	65.628	95.851	87.398	1.00	98.79	B
ATOM	2180	CA	GLY	B	159	65.143	97.215	87.309	1.00	98.79	B
ATOM	2181	C	GLY	B	159	64.874	97.567	85.857	1.00	98.79	B
ATOM	2182	O	GLY	B	159	64.864	98.739	85.477	1.00	98.79	B
ATOM	2183	N	ARG	B	160	64.670	96.533	85.044	1.00	100.00	B
ATOM	2184	CA	ARG	B	160	64.385	96.695	83.623	1.00	100.00	B
ATOM	2185	CB	ARG	B	160	64.856	95.463	82.843	1.00	100.00	B
ATOM	2186	CG	ARG	B	160	66.319	95.089	83.074	1.00	100.00	B
ATOM	2187	CD	ARG	B	160	67.266	96.199	82.645	1.00	100.00	B
ATOM	2188	NE	ARG	B	160	68.664	95.831	82.848	1.00	100.00	B
ATOM	2189	CZ	ARG	B	160	69.700	96.603	82.527	1.00	100.00	B
ATOM	2190	NH1	ARG	B	160	69.503	97.798	81.980	1.00	100.00	B
ATOM	2191	NH2	ARG	B	160	70.937	96.181	82.759	1.00	100.00	B
ATOM	2192	C	ARG	B	160	62.876	96.852	83.479	1.00	100.00	B
ATOM	2193	O	ARG	B	160	62.174	97.018	84.475	1.00	100.00	B
ATOM	2194	N	ARG	B	161	62.369	96.794	82.252	1.00	84.80	B
ATOM	2195	CA	ARG	B	161	60.934	96.941	82.043	1.00	84.80	B
ATOM	2196	CB	ARG	B	161	60.641	98.262	81.329	1.00	84.54	B
ATOM	2197	CG	ARG	B	161	60.138	99.356	82.250	1.00	84.54	B
ATOM	2198	CD	ARG	B	161	58.962	98.844	83.063	1.00	84.54	B
ATOM	2199	NE	ARG	B	161	58.217	99.902	83.739	1.00	84.54	B
ATOM	2200	CZ	ARG	B	161	58.747	100.802	84.562	1.00	84.54	B
ATOM	2201	NH1	ARG	B	161	60.049	100.794	84.826	1.00	84.54	B
ATOM	2202	NH2	ARG	B	161	57.963	101.704	85.136	1.00	84.54	B
ATOM	2203	C	ARG	B	161	60.290	95.790	81.279	1.00	84.80	B
ATOM	2204	O	ARG	B	161	60.959	95.070	80.539	1.00	84.80	B
ATOM	2205	N	TYR	B	162	58.984	95.620	81.471	1.00	99.33	B
ATOM	2206	CA	TYR	B	162	58.242	94.563	80.792	1.00	99.33	B
ATOM	2207	CB	TYR	B	162	57.028	94.124	81.623	1.00	100.00	B
ATOM	2208	CG	TYR	B	162	57.353	93.438	82.938	1.00	100.00	B
ATOM	2209	CD1	TYR	B	162	58.674	93.155	83.303	1.00	100.00	B

FIGURE 2 Continued

ATOM	2210	CE1	TYR	B	162	58.971	92.531	84.519	1.00	100.00	B
ATOM	2211	CD2	TYR	B	162	56.335	93.076	83.822	1.00	100.00	B
ATOM	2212	CE2	TYR	B	162	56.619	92.452	85.040	1.00	100.00	B
ATOM	2213	CZ	TYR	B	162	57.938	92.183	85.383	1.00	100.00	B
ATOM	2214	OH	TYR	B	162	58.222	91.582	86.592	1.00	100.00	B
ATOM	2215	C	TYR	B	162	57.765	95.068	79.436	1.00	99.33	B
ATOM	2216	O	TYR	B	162	56.669	95.618	79.320	1.00	99.33	B
ATOM	2217	N	TYR	B	163	58.590	94.873	78.412	1.00	78.76	B
ATOM	2218	CA	TYR	B	163	58.261	95.322	77.064	1.00	78.76	B
ATOM	2219	CB	TYR	B	163	59.527	95.372	76.212	1.00	72.85	B
ATOM	2220	CG	TYR	B	163	60.507	96.411	76.674	1.00	72.85	B
ATOM	2221	CD1	TYR	B	163	60.239	97.766	76.505	1.00	72.85	B
ATOM	2222	CE1	TYR	B	163	61.119	98.737	76.969	1.00	72.85	B
ATOM	2223	CD2	TYR	B	163	61.684	96.048	77.318	1.00	72.85	B
ATOM	2224	CE2	TYR	B	163	62.572	97.011	77.788	1.00	72.85	B
ATOM	2225	CZ	TYR	B	163	62.282	98.352	77.610	1.00	72.85	B
ATOM	2226	OH	TYR	B	163	63.150	99.309	78.072	1.00	72.85	B
ATOM	2227	C	TYR	B	163	57.224	94.469	76.352	1.00	78.76	B
ATOM	2228	O	TYR	B	163	57.173	93.255	76.532	1.00	78.76	B
ATOM	2229	N	VAL	B	164	56.393	95.123	75.546	1.00	77.64	B
ATOM	2230	CA	VAL	B	164	55.382	94.429	74.762	1.00	77.64	B
ATOM	2231	CB	VAL	B	164	54.337	95.413	74.198	1.00	73.41	B
ATOM	2232	CG1	VAL	B	164	53.285	94.660	73.400	1.00	73.41	B
ATOM	2233	CG2	VAL	B	164	53.689	96.180	75.331	1.00	73.41	B
ATOM	2234	C	VAL	B	164	56.169	93.814	73.609	1.00	77.64	B
ATOM	2235	O	VAL	B	164	57.190	94.367	73.191	1.00	77.64	B
ATOM	2236	N	ALA	B	165	55.721	92.677	73.093	1.00	91.04	B
ATOM	2237	CA	ALA	B	165	56.459	92.055	72.003	1.00	91.04	B
ATOM	2238	CB	ALA	B	165	57.794	91.527	72.528	1.00	97.54	B
ATOM	2239	C	ALA	B	165	55.708	90.940	71.293	1.00	91.04	B
ATOM	2240	O	ALA	B	165	54.668	90.474	71.758	1.00	91.04	B
ATOM	2241	N	LEU	B	166	56.255	90.530	70.153	1.00	99.59	B
ATOM	2242	CA	LEU	B	166	55.686	89.458	69.348	1.00	99.59	B
ATOM	2243	CB	LEU	B	166	54.923	90.031	68.151	1.00	77.78	B
ATOM	2244	CG	LEU	B	166	53.622	90.784	68.447	1.00	77.78	B
ATOM	2245	CD1	LEU	B	166	53.009	91.293	67.148	1.00	77.78	B
ATOM	2246	CD2	LEU	B	166	52.649	89.860	69.161	1.00	77.78	B
ATOM	2247	C	LEU	B	166	56.813	88.546	68.863	1.00	99.59	B
ATOM	2248	O	LEU	B	166	57.777	89.008	68.246	1.00	99.59	B
ATOM	2249	N	ASN	B	167	56.689	87.254	69.157	1.00	100.00	B
ATOM	2250	CA	ASN	B	167	57.695	86.275	68.759	1.00	100.00	B
ATOM	2251	CB	ASN	B	167	57.370	84.904	69.363	1.00	90.34	B
ATOM	2252	CG	ASN	B	167	57.493	84.888	70.882	1.00	90.34	B
ATOM	2253	OD1	ASN	B	167	58.570	85.131	71.433	1.00	90.34	B
ATOM	2254	ND2	ASN	B	167	56.389	84.601	71.563	1.00	90.34	B
ATOM	2255	C	ASN	B	167	57.782	86.171	67.242	1.00	100.00	B
ATOM	2256	O	ASN	B	167	56.869	86.596	66.529	1.00	100.00	B
ATOM	2257	N	LYS	B	168	58.882	85.602	66.753	1.00	100.00	B
ATOM	2258	CA	LYS	B	168	59.104	85.457	65.318	1.00	100.00	B
ATOM	2259	CB	LYS	B	168	60.461	84.798	65.061	1.00	100.00	B
ATOM	2260	CG	LYS	B	168	61.659	85.638	65.477	1.00	100.00	B
ATOM	2261	CD	LYS	B	168	62.957	84.989	65.012	1.00	100.00	B
ATOM	2262	CE	LYS	B	168	64.167	85.849	65.342	1.00	100.00	B
ATOM	2263	NZ	LYS	B	168	65.428	85.264	64.802	1.00	100.00	B
ATOM	2264	C	LYS	B	168	58.016	84.682	64.571	1.00	100.00	B
ATOM	2265	O	LYS	B	168	58.094	84.524	63.351	1.00	100.00	B
ATOM	2266	N	ASP	B	169	57.005	84.204	65.293	1.00	95.71	B

FIGURE 2 Continued

ATOM	2267	CA	ASP	B	169	55.920	83.454	64.665	1.00	95.71	B
ATOM	2268	CB	ASP	B	169	55.884	82.019	65.202	1.00	100.00	B
ATOM	2269	CG	ASP	B	169	55.584	81.957	66.685	1.00	100.00	B
ATOM	2270	OD1	ASP	B	169	56.304	82.615	67.467	1.00	100.00	B
ATOM	2271	OD2	ASP	B	169	54.632	81.243	67.069	1.00	100.00	B
ATOM	2272	C	ASP	B	169	54.555	84.111	64.855	1.00	95.71	B
ATOM	2273	O	ASP	B	169	53.521	83.453	64.736	1.00	95.71	B
ATOM	2274	N	GLY	B	170	54.560	85.408	65.156	1.00	100.00	B
ATOM	2275	CA	GLY	B	170	53.317	86.141	65.338	1.00	100.00	B
ATOM	2276	C	GLY	B	170	52.538	85.843	66.607	1.00	100.00	B
ATOM	2277	O	GLY	B	170	51.312	85.976	66.634	1.00	100.00	B
ATOM	2278	N	THR	B	171	53.240	85.441	67.661	1.00	100.00	B
ATOM	2279	CA	THR	B	171	52.591	85.140	68.932	1.00	100.00	B
ATOM	2280	CB	THR	B	171	52.821	83.671	69.364	1.00	99.83	B
ATOM	2281	OG1	THR	B	171	54.228	83.418	69.474	1.00	99.83	B
ATOM	2282	CG2	THR	B	171	52.209	82.712	68.356	1.00	99.83	B
ATOM	2283	C	THR	B	171	53.138	86.051	70.025	1.00	100.00	B
ATOM	2284	O	THR	B	171	54.339	86.329	70.073	1.00	100.00	B
ATOM	2285	N	PRO	B	172	52.259	86.534	70.914	1.00	89.17	B
ATOM	2286	CD	PRO	B	172	50.801	86.324	70.912	1.00	72.94	B
ATOM	2287	CA	PRO	B	172	52.661	87.417	72.013	1.00	89.17	B
ATOM	2288	CB	PRO	B	172	51.324	87.808	72.640	1.00	72.94	B
ATOM	2289	CG	PRO	B	172	50.445	86.628	72.334	1.00	72.94	B
ATOM	2290	C	PRO	B	172	53.615	86.743	73.005	1.00	89.17	B
ATOM	2291	O	PRO	B	172	53.400	85.601	73.405	1.00	89.17	B
ATOM	2292	N	ARG	B	173	54.665	87.464	73.392	1.00	79.55	B
ATOM	2293	CA	ARG	B	173	55.675	86.962	74.324	1.00	79.55	B
ATOM	2294	CB	ARG	B	173	57.052	87.492	73.897	1.00	100.00	B
ATOM	2295	CG	ARG	B	173	58.260	86.853	74.577	1.00	100.00	B
ATOM	2296	CD	ARG	B	173	59.540	87.218	73.822	1.00	100.00	B
ATOM	2297	NE	ARG	B	173	60.767	86.754	74.475	1.00	100.00	B
ATOM	2298	CZ	ARG	B	173	61.089	85.478	74.676	1.00	100.00	B
ATOM	2299	NH1	ARG	B	173	60.275	84.507	74.279	1.00	100.00	B
ATOM	2300	NH2	ARG	B	173	62.237	85.172	75.270	1.00	100.00	B
ATOM	2301	C	ARG	B	173	55.348	87.394	75.758	1.00	79.55	B
ATOM	2302	O	ARG	B	173	54.252	87.889	76.027	1.00	79.55	B
ATOM	2303	N	GLU	B	174	56.293	87.193	76.674	1.00	87.53	B
ATOM	2304	CA	GLU	B	174	56.115	87.568	78.079	1.00	87.53	B
ATOM	2305	CB	GLU	B	174	56.660	86.477	79.008	1.00	100.00	B
ATOM	2306	CG	GLU	B	174	55.764	85.260	79.186	1.00	100.00	B
ATOM	2307	CD	GLU	B	174	55.554	84.482	77.903	1.00	100.00	B
ATOM	2308	OE1	GLU	B	174	56.560	84.107	77.259	1.00	100.00	B
ATOM	2309	OE2	GLU	B	174	54.381	84.238	77.545	1.00	100.00	B
ATOM	2310	C	GLU	B	174	56.838	88.873	78.389	1.00	87.53	B
ATOM	2311	O	GLU	B	174	58.006	89.042	78.031	1.00	87.53	B
ATOM	2312	N	GLY	B	175	56.144	89.787	79.062	1.00	84.47	B
ATOM	2313	CA	GLY	B	175	56.747	91.062	79.409	1.00	84.47	B
ATOM	2314	C	GLY	B	175	58.057	90.849	80.136	1.00	84.47	B
ATOM	2315	O	GLY	B	175	58.996	91.642	80.023	1.00	84.47	B
ATOM	2316	N	THR	B	176	58.115	89.751	80.878	1.00	99.28	B
ATOM	2317	CA	THR	B	176	59.290	89.382	81.653	1.00	99.28	B
ATOM	2318	CB	THR	B	176	58.929	88.287	82.656	1.00	99.44	B
ATOM	2319	OG1	THR	B	176	58.365	87.174	81.950	1.00	99.44	B
ATOM	2320	CG2	THR	B	176	57.913	88.804	83.664	1.00	99.44	B
ATOM	2321	C	THR	B	176	60.419	88.867	80.765	1.00	99.28	B
ATOM	2322	O	THR	B	176	61.601	89.040	81.076	1.00	99.28	B
ATOM	2323	N	ARG	B	177	60.043	88.234	79.658	1.00	100.00	B

FIGURE 2 Continued

ATOM	2324	CA	ARG	B	177	61.009	87.672	78.723	1.00	100.00	B
ATOM	2325	CB	ARG	B	177	60.447	86.378	78.121	1.00	100.00	B
ATOM	2326	CG	ARG	B	177	60.135	85.295	79.151	1.00	100.00	B
ATOM	2327	CD	ARG	B	177	59.506	84.063	78.509	1.00	100.00	B
ATOM	2328	NE	ARG	B	177	60.360	83.475	77.477	1.00	100.00	B
ATOM	2329	CZ	ARG	B	177	60.046	82.392	76.769	1.00	100.00	B
ATOM	2330	NH1	ARG	B	177	58.892	81.771	76.981	1.00	100.00	B
ATOM	2331	NH2	ARG	B	177	60.882	81.933	75.844	1.00	100.00	B
ATOM	2332	C	ARG	B	177	61.398	88.635	77.599	1.00	100.00	B
ATOM	2333	O	ARG	B	177	61.624	88.209	76.466	1.00	100.00	B
ATOM	2334	N	THR	B	178	61.489	89.925	77.908	1.00	99.59	B
ATOM	2335	CA	THR	B	178	61.848	90.914	76.894	1.00	99.59	B
ATOM	2336	CB	THR	B	178	60.604	91.661	76.380	1.00	95.63	B
ATOM	2337	OG1	THR	B	178	59.917	92.260	77.485	1.00	95.63	B
ATOM	2338	CG2	THR	B	178	59.665	90.709	75.659	1.00	95.63	B
ATOM	2339	C	THR	B	178	62.854	91.961	77.362	1.00	99.59	B
ATOM	2340	O	THR	B	178	62.992	92.233	78.556	1.00	99.59	B
ATOM	2341	N	LYS	B	179	63.553	92.544	76.393	1.00	93.31	B
ATOM	2342	CA	LYS	B	179	64.544	93.580	76.649	1.00	93.31	B
ATOM	2343	CB	LYS	B	179	65.941	92.970	76.791	1.00	99.69	B
ATOM	2344	CG	LYS	B	179	66.140	92.164	78.060	1.00	99.69	B
ATOM	2345	CD	LYS	B	179	67.596	91.758	78.236	1.00	99.69	B
ATOM	2346	CE	LYS	B	179	67.807	91.051	79.567	1.00	99.69	B
ATOM	2347	NZ	LYS	B	179	69.226	90.645	79.770	1.00	99.69	B
ATOM	2348	C	LYS	B	179	64.548	94.587	75.503	1.00	93.31	B
ATOM	2349	O	LYS	B	179	64.225	94.246	74.364	1.00	93.31	B
ATOM	2350	N	ARG	B	180	64.905	95.830	75.811	1.00	100.00	B
ATOM	2351	CA	ARG	B	180	64.962	96.881	74.802	1.00	100.00	B
ATOM	2352	CB	ARG	B	180	65.285	98.229	75.460	1.00	89.36	B
ATOM	2353	CG	ARG	B	180	65.024	99.444	74.580	1.00	89.36	B
ATOM	2354	CD	ARG	B	180	65.872	100.654	74.989	1.00	89.36	B
ATOM	2355	NE	ARG	B	180	65.615	101.150	76.343	1.00	89.36	B
ATOM	2356	CZ	ARG	B	180	64.507	101.778	76.728	1.00	89.36	B
ATOM	2357	NH1	ARG	B	180	63.521	101.998	75.867	1.00	89.36	B
ATOM	2358	NH2	ARG	B	180	64.388	102.204	77.978	1.00	89.36	B
ATOM	2359	C	ARG	B	180	66.079	96.504	73.835	1.00	100.00	B
ATOM	2360	O	ARG	B	180	66.893	95.628	74.131	1.00	100.00	B
ATOM	2361	N	HIS	B	181	66.115	97.155	72.678	1.00	99.13	B
ATOM	2362	CA	HIS	B	181	67.155	96.888	71.689	1.00	99.13	B
ATOM	2363	CB	HIS	B	181	68.531	97.000	72.348	1.00	100.00	B
ATOM	2364	CG	HIS	B	181	68.758	98.306	73.044	1.00	100.00	B
ATOM	2365	CD2	HIS	B	181	68.160	99.512	72.894	1.00	100.00	B
ATOM	2366	ND1	HIS	B	181	69.708	98.470	74.030	1.00	100.00	B
ATOM	2367	CE1	HIS	B	181	69.683	99.720	74.459	1.00	100.00	B
ATOM	2368	NE2	HIS	B	181	68.752	100.373	73.786	1.00	100.00	B
ATOM	2369	C	HIS	B	181	67.005	95.519	71.034	1.00	99.13	B
ATOM	2370	O	HIS	B	181	67.937	95.022	70.403	1.00	99.13	B
ATOM	2371	N	GLN	B	182	65.832	94.913	71.185	1.00	99.52	B
ATOM	2372	CA	GLN	B	182	65.567	93.609	70.589	1.00	99.52	B
ATOM	2373	CB	GLN	B	182	65.279	92.576	71.674	1.00	100.00	B
ATOM	2374	CG	GLN	B	182	66.446	92.349	72.615	1.00	100.00	B
ATOM	2375	CD	GLN	B	182	66.240	91.150	73.514	1.00	100.00	B
ATOM	2376	OE1	GLN	B	182	65.276	91.087	74.281	1.00	100.00	B
ATOM	2377	NE2	GLN	B	182	67.149	90.185	73.424	1.00	100.00	B
ATOM	2378	C	GLN	B	182	64.394	93.687	69.619	1.00	99.52	B
ATOM	2379	O	GLN	B	182	63.264	93.978	70.010	1.00	99.52	B
ATOM	2380	N	LYS	B	183	64.682	93.415	68.352	1.00	97.95	B

FIGURE 2 Continued

ATOM	2381	CA	LYS	B	183	63.693	93.469	67.285	1.00	97.95	B
ATOM	2382	CB	LYS	B	183	64.179	92.652	66.079	1.00	100.00	B
ATOM	2383	CG	LYS	B	183	65.331	93.306	65.306	1.00	100.00	B
ATOM	2384	CD	LYS	B	183	65.524	92.667	63.929	1.00	100.00	B
ATOM	2385	CE	LYS	B	183	66.523	93.446	63.073	1.00	100.00	B
ATOM	2386	NZ	LYS	B	183	66.572	92.945	61.666	1.00	100.00	B
ATOM	2387	C	LYS	B	183	62.257	93.072	67.623	1.00	97.95	B
ATOM	2388	O	LYS	B	183	61.322	93.648	67.070	1.00	97.95	B
ATOM	2389	N	PHE	B	184	62.057	92.108	68.518	1.00	79.35	B
ATOM	2390	CA	PHE	B	184	60.687	91.709	68.840	1.00	79.35	B
ATOM	2391	CB	PHE	B	184	60.639	90.276	69.407	1.00	99.94	B
ATOM	2392	CG	PHE	B	184	61.534	90.043	70.595	1.00	99.94	B
ATOM	2393	CD1	PHE	B	184	62.917	89.946	70.441	1.00	99.94	B
ATOM	2394	CD2	PHE	B	184	60.991	89.890	71.870	1.00	99.94	B
ATOM	2395	CE1	PHE	B	184	63.744	89.695	71.539	1.00	99.94	B
ATOM	2396	CE2	PHE	B	184	61.809	89.640	72.974	1.00	99.94	B
ATOM	2397	CZ	PHE	B	184	63.187	89.542	72.809	1.00	99.94	B
ATOM	2398	C	PHE	B	184	59.947	92.678	69.771	1.00	79.35	B
ATOM	2399	O	PHE	B	184	58.732	92.570	69.951	1.00	79.35	B
ATOM	2400	N	THR	B	185	60.674	93.632	70.348	1.00	100.00	B
ATOM	2401	CA	THR	B	185	60.067	94.620	71.240	1.00	100.00	B
ATOM	2402	CB	THR	B	185	60.911	94.829	72.514	1.00	99.28	B
ATOM	2403	OG1	THR	B	185	62.194	95.360	72.156	1.00	99.28	B
ATOM	2404	CG2	THR	B	185	61.093	93.513	73.258	1.00	99.28	B
ATOM	2405	C	THR	B	185	59.952	95.966	70.531	1.00	100.00	B
ATOM	2406	O	THR	B	185	59.541	96.961	71.130	1.00	100.00	B
ATOM	2407	N	HIS	B	186	60.317	95.980	69.251	1.00	80.24	B
ATOM	2408	CA	HIS	B	186	60.284	97.192	68.439	1.00	80.24	B
ATOM	2409	CB	HIS	B	186	61.568	97.296	67.617	1.00	86.10	B
ATOM	2410	CG	HIS	B	186	62.816	97.258	68.442	1.00	86.10	B
ATOM	2411	CD2	HIS	B	186	63.000	97.110	69.776	1.00	86.10	B
ATOM	2412	ND1	HIS	B	186	64.074	97.380	67.893	1.00	86.10	B
ATOM	2413	CE1	HIS	B	186	64.980	97.309	68.853	1.00	86.10	B
ATOM	2414	NE2	HIS	B	186	64.354	97.145	70.005	1.00	86.10	B
ATOM	2415	C	HIS	B	186	59.079	97.241	67.508	1.00	80.24	B
ATOM	2416	O	HIS	B	186	58.871	96.344	66.685	1.00	80.24	B
ATOM	2417	N	PHE	B	187	58.284	98.298	67.642	1.00	64.76	B
ATOM	2418	CA	PHE	B	187	57.103	98.454	66.813	1.00	64.76	B
ATOM	2419	CB	PHE	B	187	55.835	98.348	67.657	1.00	68.83	B
ATOM	2420	CG	PHE	B	187	55.606	96.985	68.232	1.00	68.83	B
ATOM	2421	CD1	PHE	B	187	56.423	96.496	69.249	1.00	68.83	B
ATOM	2422	CD2	PHE	B	187	54.570	96.185	67.758	1.00	68.83	B
ATOM	2423	CE1	PHE	B	187	56.209	95.229	69.786	1.00	68.83	B
ATOM	2424	CE2	PHE	B	187	54.347	94.914	68.289	1.00	68.83	B
ATOM	2425	CZ	PHE	B	187	55.167	94.436	69.304	1.00	68.83	B
ATOM	2426	C	PHE	B	187	57.099	99.770	66.054	1.00	64.76	B
ATOM	2427	O	PHE	B	187	57.579	100.797	66.542	1.00	64.76	B
ATOM	2428	N	LEU	B	188	56.542	99.718	64.850	1.00	62.18	B
ATOM	2429	CA	LEU	B	188	56.456	100.875	63.981	1.00	62.18	B
ATOM	2430	CB	LEU	B	188	57.089	100.555	62.625	1.00	63.11	B
ATOM	2431	CG	LEU	B	188	56.835	101.541	61.488	1.00	63.11	B
ATOM	2432	CD1	LEU	B	188	57.459	102.884	61.823	1.00	63.11	B
ATOM	2433	CD2	LEU	B	188	57.406	100.977	60.197	1.00	63.11	B
ATOM	2434	C	LEU	B	188	55.009	101.291	63.776	1.00	62.18	B
ATOM	2435	O	LEU	B	188	54.206	100.548	63.217	1.00	62.18	B
ATOM	2436	N	PRO	B	189	54.651	102.486	64.245	1.00	54.68	B
ATOM	2437	CD	PRO	B	189	55.379	103.405	65.135	1.00	51.12	B

FIGURE 2 Continued

ATOM	2438	CA	PRO	B	189	53.267	102.913	64.053	1.00	54.68	B
ATOM	2439	CB	PRO	B	189	53.173	104.176	64.901	1.00	51.12	B
ATOM	2440	CG	PRO	B	189	54.262	103.981	65.949	1.00	51.12	B
ATOM	2441	C	PRO	B	189	53.106	103.206	62.567	1.00	54.68	B
ATOM	2442	O	PRO	B	189	53.826	104.040	62.018	1.00	54.68	B
ATOM	2443	N	ARG	B	190	52.185	102.509	61.915	1.00	58.99	B
ATOM	2444	CA	ARG	B	190	51.957	102.712	60.491	1.00	58.99	B
ATOM	2445	CB	ARG	B	190	51.990	101.370	59.746	1.00	52.79	B
ATOM	2446	CG	ARG	B	190	53.355	100.690	59.722	1.00	52.79	B
ATOM	2447	CD	ARG	B	190	53.365	99.514	58.742	1.00	52.79	B
ATOM	2448	NE	ARG	B	190	52.927	99.934	57.414	1.00	52.79	B
ATOM	2449	CZ	ARG	B	190	51.954	99.342	56.729	1.00	52.79	B
ATOM	2450	NH1	ARG	B	190	51.319	98.296	57.241	1.00	52.79	B
ATOM	2451	NH2	ARG	B	190	51.596	99.813	55.542	1.00	52.79	B
ATOM	2452	C	ARG	B	190	50.619	103.401	60.257	1.00	58.99	B
ATOM	2453	O	ARG	B	190	49.707	103.300	61.068	1.00	58.99	B
ATOM	2454	N	PRO	B	191	50.489	104.116	59.135	1.00	67.02	B
ATOM	2455	CD	PRO	B	191	51.515	104.360	58.108	1.00	45.04	B
ATOM	2456	CA	PRO	B	191	49.255	104.821	58.801	1.00	67.02	B
ATOM	2457	CB	PRO	B	191	49.708	105.784	57.714	1.00	45.04	B
ATOM	2458	CG	PRO	B	191	50.708	104.985	56.991	1.00	45.04	B
ATOM	2459	C	PRO	B	191	48.174	103.869	58.311	1.00	67.02	B
ATOM	2460	O	PRO	B	191	48.447	102.719	57.972	1.00	67.02	B
ATOM	2461	N	VAL	B	192	46.942	104.351	58.274	1.00	60.09	B
ATOM	2462	CA	VAL	B	192	45.843	103.528	57.814	1.00	60.09	B
ATOM	2463	CB	VAL	B	192	44.784	103.350	58.912	1.00	63.89	B
ATOM	2464	CG1	VAL	B	192	43.629	102.525	58.390	1.00	63.89	B
ATOM	2465	CG2	VAL	B	192	45.402	102.668	60.113	1.00	63.89	B
ATOM	2466	C	VAL	B	192	45.201	104.159	56.589	1.00	60.09	B
ATOM	2467	O	VAL	B	192	44.847	105.342	56.590	1.00	60.09	B
ATOM	2468	N	ASP	B	193	45.077	103.362	55.534	1.00	60.03	B
ATOM	2469	CA	ASP	B	193	44.471	103.813	54.292	1.00	60.03	B
ATOM	2470	CB	ASP	B	193	44.914	102.907	53.142	1.00	83.98	B
ATOM	2471	CG	ASP	B	193	44.253	103.259	51.824	1.00	83.98	B
ATOM	2472	OD1	ASP	B	193	44.487	102.523	50.847	1.00	83.98	B
ATOM	2473	OD2	ASP	B	193	43.506	104.260	51.756	1.00	83.98	B
ATOM	2474	C	ASP	B	193	42.965	103.724	54.478	1.00	60.03	B
ATOM	2475	O	ASP	B	193	42.434	102.656	54.774	1.00	60.03	B
ATOM	2476	N	PRO	B	194	42.254	104.849	54.313	1.00	84.27	B
ATOM	2477	CD	PRO	B	194	42.729	106.179	53.889	1.00	72.99	B
ATOM	2478	CA	PRO	B	194	40.797	104.832	54.479	1.00	84.27	B
ATOM	2479	CB	PRO	B	194	40.409	106.293	54.244	1.00	72.99	B
ATOM	2480	CG	PRO	B	194	41.484	106.785	53.295	1.00	72.99	B
ATOM	2481	C	PRO	B	194	40.095	103.867	53.518	1.00	84.27	B
ATOM	2482	O	PRO	B	194	39.174	103.147	53.908	1.00	84.27	B
ATOM	2483	N	ASP	B	195	40.546	103.853	52.267	1.00	83.93	B
ATOM	2484	CA	ASP	B	195	39.971	102.992	51.237	1.00	83.93	B
ATOM	2485	CB	ASP	B	195	40.694	103.207	49.907	1.00	100.00	B
ATOM	2486	CG	ASP	B	195	40.795	104.668	49.526	1.00	100.00	B
ATOM	2487	OD1	ASP	B	195	39.737	105.313	49.358	1.00	100.00	B
ATOM	2488	OD2	ASP	B	195	41.935	105.169	49.395	1.00	100.00	B
ATOM	2489	C	ASP	B	195	40.062	101.514	51.605	1.00	83.93	B
ATOM	2490	O	ASP	B	195	39.159	100.736	51.305	1.00	83.93	B
ATOM	2491	N	LYS	B	196	41.160	101.128	52.248	1.00	73.50	B
ATOM	2492	CA	LYS	B	196	41.361	99.740	52.633	1.00	73.50	B
ATOM	2493	CB	LYS	B	196	42.852	99.465	52.826	1.00	99.37	B
ATOM	2494	CG	LYS	B	196	43.630	99.418	51.525	1.00	99.37	B

FIGURE 2 Continued

ATOM	2495	CD	LYS	B	196	45.082	99.037	51.760	1.00	99.37	B
ATOM	2496	CE	LYS	B	196	45.789	98.742	50.446	1.00	99.37	B
ATOM	2497	NZ	LYS	B	196	45.161	97.591	49.733	1.00	99.37	B
ATOM	2498	C	LYS	B	196	40.585	99.311	53.873	1.00	73.50	B
ATOM	2499	O	LYS	B	196	40.554	98.129	54.211	1.00	73.50	B
ATOM	2500	N	VAL	B	197	39.954	100.269	54.547	1.00	99.89	B
ATOM	2501	CA	VAL	B	197	39.169	99.972	55.743	1.00	99.89	B
ATOM	2502	CB	VAL	B	197	39.764	100.667	56.988	1.00	99.57	B
ATOM	2503	CG1	VAL	B	197	41.059	99.978	57.403	1.00	99.57	B
ATOM	2504	CG2	VAL	B	197	40.025	102.136	56.687	1.00	99.57	B
ATOM	2505	C	VAL	B	197	37.718	100.415	55.553	1.00	99.89	B
ATOM	2506	O	VAL	B	197	37.332	101.516	55.943	1.00	99.89	B
ATOM	2507	N	PRO	B	198	36.893	99.549	54.950	1.00	82.81	B
ATOM	2508	CD	PRO	B	198	37.264	98.203	54.477	1.00	78.19	B
ATOM	2509	CA	PRO	B	198	35.477	99.821	54.687	1.00	82.81	B
ATOM	2510	CB	PRO	B	198	35.045	98.609	53.862	1.00	78.19	B
ATOM	2511	CG	PRO	B	198	35.927	97.518	54.383	1.00	78.19	B
ATOM	2512	C	PRO	B	198	34.602	100.035	55.925	1.00	82.81	B
ATOM	2513	O	PRO	B	198	33.521	100.616	55.832	1.00	82.81	B
ATOM	2514	N	GLU	B	199	35.065	99.570	57.079	1.00	99.54	B
ATOM	2515	CA	GLU	B	199	34.305	99.731	58.317	1.00	99.54	B
ATOM	2516	CB	GLU	B	199	34.568	98.545	59.245	1.00	100.00	B
ATOM	2517	CG	GLU	B	199	34.128	97.214	58.665	1.00	100.00	B
ATOM	2518	CD	GLU	B	199	32.638	97.177	58.378	1.00	100.00	B
ATOM	2519	OE1	GLU	B	199	31.846	97.254	59.344	1.00	100.00	B
ATOM	2520	OE2	GLU	B	199	32.261	97.077	57.189	1.00	100.00	B
ATOM	2521	C	GLU	B	199	34.704	101.030	59.008	1.00	99.54	B
ATOM	2522	O	GLU	B	199	35.006	101.048	60.205	1.00	99.54	B
ATOM	2523	N	LEU	B	200	34.689	102.119	58.247	1.00	78.12	B
ATOM	2524	CA	LEU	B	200	35.084	103.418	58.768	1.00	78.12	B
ATOM	2525	CB	LEU	B	200	36.532	103.716	58.340	1.00	69.43	B
ATOM	2526	CG	LEU	B	200	37.188	105.059	58.688	1.00	69.43	B
ATOM	2527	CD1	LEU	B	200	38.649	104.833	59.068	1.00	69.43	B
ATOM	2528	CD2	LEU	B	200	37.066	106.014	57.509	1.00	69.43	B
ATOM	2529	C	LEU	B	200	34.156	104.529	58.303	1.00	78.12	B
ATOM	2530	O	LEU	B	200	34.094	105.590	58.921	1.00	78.12	B
ATOM	2531	N	TYR	B	201	33.437	104.292	57.211	1.00	90.96	B
ATOM	2532	CA	TYR	B	201	32.522	105.302	56.696	1.00	90.96	B
ATOM	2533	CB	TYR	B	201	32.059	104.934	55.279	1.00	88.44	B
ATOM	2534	CG	TYR	B	201	31.016	103.834	55.196	1.00	88.44	B
ATOM	2535	CD1	TYR	B	201	29.654	104.123	55.318	1.00	88.44	B
ATOM	2536	CE1	TYR	B	201	28.687	103.116	55.225	1.00	88.44	B
ATOM	2537	CD2	TYR	B	201	31.388	102.507	54.983	1.00	88.44	B
ATOM	2538	CE2	TYR	B	201	30.432	101.491	54.889	1.00	88.44	B
ATOM	2539	CZ	TYR	B	201	29.085	101.800	55.009	1.00	88.44	B
ATOM	2540	OH	TYR	B	201	28.141	100.796	54.906	1.00	88.44	B
ATOM	2541	C	TYR	B	201	31.339	105.398	57.651	1.00	90.96	B
ATOM	2542	O	TYR	B	201	30.586	106.370	57.633	1.00	90.96	B
ATOM	2543	N	LYS	B	202	31.197	104.378	58.494	1.00	87.19	B
ATOM	2544	CA	LYS	B	202	30.124	104.322	59.479	1.00	87.19	B
ATOM	2545	CB	LYS	B	202	30.031	102.915	60.069	1.00	99.99	B
ATOM	2546	CG	LYS	B	202	29.805	101.827	59.033	1.00	99.99	B
ATOM	2547	CD	LYS	B	202	29.721	100.452	59.679	1.00	99.99	B
ATOM	2548	CE	LYS	B	202	29.500	99.363	58.640	1.00	99.99	B
ATOM	2549	NZ	LYS	B	202	30.612	99.310	57.647	1.00	99.99	B
ATOM	2550	C	LYS	B	202	30.398	105.329	60.591	1.00	87.19	B
ATOM	2551	O	LYS	B	202	29.474	105.849	61.220	1.00	87.19	B

FIGURE 2 Continued

ATOM	2552	N	ASP	B	203	31.677	105.600	60.827	1.00	98.64	B
ATOM	2553	CA	ASP	B	203	32.076	106.548	61.856	1.00	98.64	B
ATOM	2554	CB	ASP	B	203	33.397	106.111	62.494	1.00	91.68	B
ATOM	2555	CG	ASP	B	203	33.460	104.613	62.739	1.00	91.68	B
ATOM	2556	OD1	ASP	B	203	32.495	104.055	63.302	1.00	91.68	B
ATOM	2557	OD2	ASP	B	203	34.480	103.992	62.371	1.00	91.68	B
ATOM	2558	C	ASP	B	203	32.243	107.921	61.222	1.00	98.64	B
ATOM	2559	O	ASP	B	203	32.531	108.899	61.911	1.00	98.64	B
ATOM	2560	N	ILE	B	204	32.054	107.986	59.906	1.00	81.26	B
ATOM	2561	CA	ILE	B	204	32.197	109.237	59.163	1.00	81.26	B
ATOM	2562	CB	ILE	B	204	33.100	109.058	57.923	1.00	98.99	B
ATOM	2563	CG2	ILE	B	204	33.205	110.373	57.167	1.00	98.99	B
ATOM	2564	CG1	ILE	B	204	34.481	108.543	58.337	1.00	98.99	B
ATOM	2565	CD1	ILE	B	204	35.263	109.491	59.213	1.00	98.99	B
ATOM	2566	C	ILE	B	204	30.859	109.769	58.665	1.00	81.26	B
ATOM	2567	O	ILE	B	204	30.500	110.918	58.915	1.00	81.26	B
ATOM	2568	N	LEU	B	205	30.133	108.924	57.944	1.00	91.26	B
ATOM	2569	CA	LEU	B	205	28.840	109.294	57.382	1.00	91.26	B
ATOM	2570	CB	LEU	B	205	28.570	108.461	56.129	1.00	88.77	B
ATOM	2571	CG	LEU	B	205	29.624	108.529	55.025	1.00	88.77	B
ATOM	2572	CD1	LEU	B	205	29.351	107.437	54.000	1.00	88.77	B
ATOM	2573	CD2	LEU	B	205	29.608	109.909	54.383	1.00	88.77	B
ATOM	2574	C	LEU	B	205	27.698	109.096	58.372	1.00	91.26	B
ATOM	2575	O	LEU	B	205	27.686	108.133	59.140	1.00	91.26	B
ATOM	2576	N	SER	B	206	26.736	110.011	58.352	1.00	82.87	B
ATOM	2577	CA	SER	B	206	25.596	109.894	59.245	1.00	82.87	B
ATOM	2578	CB	SER	B	206	24.750	111.167	59.209	1.00	68.58	B
ATOM	2579	OG	SER	B	206	24.209	111.391	57.923	1.00	68.58	B
ATOM	2580	C	SER	B	206	24.786	108.702	58.761	1.00	82.87	B
ATOM	2581	O	SER	B	206	24.778	108.396	57.570	1.00	82.87	B
ATOM	2582	N	GLN	B	207	24.115	108.020	59.679	1.00	90.75	B
ATOM	2583	CA	GLN	B	207	23.322	106.854	59.317	1.00	90.75	B
ATOM	2584	CB	GLN	B	207	22.894	106.115	60.587	1.00	100.00	B
ATOM	2585	CG	GLN	B	207	22.140	104.821	60.349	1.00	100.00	B
ATOM	2586	CD	GLN	B	207	21.829	104.082	61.638	1.00	100.00	B
ATOM	2587	OE1	GLN	B	207	21.131	103.066	61.632	1.00	100.00	B
ATOM	2588	NE2	GLN	B	207	22.351	104.587	62.753	1.00	100.00	B
ATOM	2589	C	GLN	B	207	22.097	107.246	58.488	1.00	90.75	B
ATOM	2590	O	GLN	B	207	21.749	108.450	58.459	1.00	90.75	B
ATOM	2591	OXT	GLN	B	207	21.497	106.338	57.875	1.00	99.88	B
ATOM	2592	CB	THR	C	52	32.968	119.253	55.113	1.00	100.00	C
ATOM	2593	OG1	THR	C	52	33.012	118.160	56.042	1.00	100.00	C
ATOM	2594	CG2	THR	C	52	33.207	120.570	55.857	1.00	100.00	C
ATOM	2595	C	THR	C	52	31.499	118.066	53.456	1.00	99.97	C
ATOM	2596	O	THR	C	52	30.536	117.298	53.510	1.00	99.97	C
ATOM	2597	N	THR	C	52	30.479	119.295	55.385	1.00	99.97	C
ATOM	2598	CA	THR	C	52	31.594	119.273	54.396	1.00	99.97	C
ATOM	2599	N	ASP	C	53	32.506	117.909	52.598	1.00	100.00	C
ATOM	2600	CA	ASP	C	53	32.553	116.813	51.630	1.00	100.00	C
ATOM	2601	CB	ASP	C	53	33.302	117.272	50.376	1.00	100.00	C
ATOM	2602	CG	ASP	C	53	33.064	116.366	49.186	1.00	100.00	C
ATOM	2603	OD1	ASP	C	53	33.748	116.557	48.156	1.00	100.00	C
ATOM	2604	OD2	ASP	C	53	32.190	115.473	49.275	1.00	100.00	C
ATOM	2605	C	ASP	C	53	33.239	115.573	52.214	1.00	100.00	C
ATOM	2606	O	ASP	C	53	33.900	115.651	53.253	1.00	100.00	C
ATOM	2607	N	LEU	C	54	33.083	114.433	51.543	1.00	94.05	C
ATOM	2608	CA	LEU	C	54	33.689	113.183	52.004	1.00	94.05	C

FIGURE 2 Continued

ATOM	2609	CB	LEU	C	54	32.818	111.987	51.617	1.00	97.96	C
ATOM	2610	CG	LEU	C	54	33.439	110.619	51.915	1.00	97.96	C
ATOM	2611	CD1	LEU	C	54	33.779	110.524	53.393	1.00	97.96	C
ATOM	2612	CD2	LEU	C	54	32.479	109.516	51.511	1.00	97.96	C
ATOM	2613	C	LEU	C	54	35.087	112.980	51.435	1.00	94.05	C
ATOM	2614	O	LEU	C	54	35.987	112.497	52.125	1.00	94.05	C
ATOM	2615	N	ASP	C	55	35.258	113.335	50.166	1.00	89.17	C
ATOM	2616	CA	ASP	C	55	36.551	113.209	49.510	1.00	89.17	C
ATOM	2617	CB	ASP	C	55	36.431	113.662	48.056	1.00	100.00	C
ATOM	2618	CG	ASP	C	55	35.196	113.092	47.372	1.00	100.00	C
ATOM	2619	OD1	ASP	C	55	35.071	111.850	47.296	1.00	100.00	C
ATOM	2620	OD2	ASP	C	55	34.345	113.888	46.916	1.00	100.00	C
ATOM	2621	C	ASP	C	55	37.514	114.108	50.281	1.00	89.17	C
ATOM	2622	O	ASP	C	55	38.706	113.825	50.392	1.00	89.17	C
ATOM	2623	N	HIS	C	56	36.965	115.194	50.816	1.00	75.92	C
ATOM	2624	CA	HIS	C	56	37.714	116.159	51.611	1.00	75.92	C
ATOM	2625	CB	HIS	C	56	36.745	117.220	52.154	1.00	100.00	C
ATOM	2626	CG	HIS	C	56	37.360	118.182	53.124	1.00	100.00	C
ATOM	2627	CD2	HIS	C	56	38.651	118.529	53.349	1.00	100.00	C
ATOM	2628	ND1	HIS	C	56	36.604	118.940	53.995	1.00	100.00	C
ATOM	2629	CE1	HIS	C	56	37.402	119.710	54.713	1.00	100.00	C
ATOM	2630	NE2	HIS	C	56	38.649	119.480	54.341	1.00	100.00	C
ATOM	2631	C	HIS	C	56	38.370	115.420	52.774	1.00	75.92	C
ATOM	2632	O	HIS	C	56	39.580	115.502	52.986	1.00	75.92	C
ATOM	2633	N	LEU	C	57	37.551	114.684	53.514	1.00	68.76	C
ATOM	2634	CA	LEU	C	57	38.017	113.941	54.674	1.00	68.76	C
ATOM	2635	CB	LEU	C	57	36.823	113.378	55.442	1.00	80.51	C
ATOM	2636	CG	LEU	C	57	37.174	112.729	56.779	1.00	80.51	C
ATOM	2637	CD1	LEU	C	57	37.923	113.723	57.660	1.00	80.51	C
ATOM	2638	CD2	LEU	C	57	35.903	112.267	57.462	1.00	80.51	C
ATOM	2639	C	LEU	C	57	38.986	112.814	54.349	1.00	68.76	C
ATOM	2640	O	LEU	C	57	39.910	112.545	55.115	1.00	68.76	C
ATOM	2641	N	LYS	C	58	38.776	112.142	53.223	1.00	61.74	C
ATOM	2642	CA	LYS	C	58	39.668	111.049	52.851	1.00	61.74	C
ATOM	2643	CB	LYS	C	58	39.135	110.311	51.619	1.00	84.68	C
ATOM	2644	CG	LYS	C	58	37.715	109.800	51.806	1.00	84.68	C
ATOM	2645	CD	LYS	C	58	37.331	108.750	50.781	1.00	84.68	C
ATOM	2646	CE	LYS	C	58	37.964	107.407	51.101	1.00	84.68	C
ATOM	2647	NZ	LYS	C	58	37.508	106.360	50.146	1.00	84.68	C
ATOM	2648	C	LYS	C	58	41.058	111.611	52.588	1.00	61.74	C
ATOM	2649	O	LYS	C	58	42.060	110.956	52.872	1.00	61.74	C
ATOM	2650	N	GLY	C	59	41.102	112.836	52.063	1.00	57.71	C
ATOM	2651	CA	GLY	C	59	42.370	113.489	51.788	1.00	57.71	C
ATOM	2652	C	GLY	C	59	43.141	113.657	53.082	1.00	57.71	C
ATOM	2653	O	GLY	C	59	44.309	113.280	53.182	1.00	57.71	C
ATOM	2654	N	ILE	C	60	42.466	114.217	54.079	1.00	57.00	C
ATOM	2655	CA	ILE	C	60	43.039	114.435	55.399	1.00	57.00	C
ATOM	2656	CB	ILE	C	60	41.997	115.096	56.310	1.00	56.02	C
ATOM	2657	CG2	ILE	C	60	42.558	115.296	57.706	1.00	56.02	C
ATOM	2658	CG1	ILE	C	60	41.579	116.428	55.689	1.00	56.02	C
ATOM	2659	CD1	ILE	C	60	40.350	117.025	56.286	1.00	56.02	C
ATOM	2660	C	ILE	C	60	43.503	113.113	56.013	1.00	57.00	C
ATOM	2661	O	ILE	C	60	44.468	113.076	56.776	1.00	57.00	C
ATOM	2662	N	LEU	C	61	42.813	112.029	55.677	1.00	59.72	C
ATOM	2663	CA	LEU	C	61	43.182	110.715	56.185	1.00	59.72	C
ATOM	2664	CB	LEU	C	61	42.000	109.742	56.071	1.00	56.09	C
ATOM	2665	CG	LEU	C	61	40.726	110.076	56.856	1.00	56.09	C

FIGURE 2 Continued

ATOM	2666	CD1	LEU	C	61	39.705	108.981	56.667	1.00	56.09	C
ATOM	2667	CD2	LEU	C	61	41.057	110.229	58.328	1.00	56.09	C
ATOM	2668	C	LEU	C	61	44.381	110.170	55.404	1.00	59.72	C
ATOM	2669	O	LEU	C	61	45.073	109.259	55.864	1.00	59.72	C
ATOM	2670	N	ARG	C	62	44.620	110.730	54.220	1.00	57.36	C
ATOM	2671	CA	ARG	C	62	45.740	110.302	53.384	1.00	57.36	C
ATOM	2672	CB	ARG	C	62	45.376	110.386	51.897	1.00	67.53	C
ATOM	2673	CG	ARG	C	62	44.179	109.547	51.501	1.00	67.53	C
ATOM	2674	CD	ARG	C	62	44.415	108.825	50.196	1.00	67.53	C
ATOM	2675	NE	ARG	C	62	43.243	108.058	49.779	1.00	67.53	C
ATOM	2676	CZ	ARG	C	62	42.127	108.597	49.291	1.00	67.53	C
ATOM	2677	NH1	ARG	C	62	42.023	109.914	49.154	1.00	67.53	C
ATOM	2678	NH2	ARG	C	62	41.116	107.818	48.934	1.00	67.53	C
ATOM	2679	C	ARG	C	62	46.992	111.137	53.645	1.00	57.36	C
ATOM	2680	O	ARG	C	62	47.933	111.119	52.853	1.00	57.36	C
ATOM	2681	N	ARG	C	63	46.996	111.867	54.757	1.00	47.93	C
ATOM	2682	CA	ARG	C	63	48.142	112.687	55.123	1.00	47.93	C
ATOM	2683	CB	ARG	C	63	47.704	113.846	56.013	1.00	49.06	C
ATOM	2684	CG	ARG	C	63	46.906	114.867	55.234	1.00	49.06	C
ATOM	2685	CD	ARG	C	63	46.564	116.077	56.056	1.00	49.06	C
ATOM	2686	NE	ARG	C	63	45.807	117.037	55.265	1.00	49.06	C
ATOM	2687	CZ	ARG	C	63	45.412	118.224	55.711	1.00	49.06	C
ATOM	2688	NH1	ARG	C	63	45.700	118.606	56.950	1.00	49.06	C
ATOM	2689	NH2	ARG	C	63	44.741	119.037	54.912	1.00	49.06	C
ATOM	2690	C	ARG	C	63	49.225	111.855	55.805	1.00	47.93	C
ATOM	2691	O	ARG	C	63	48.957	111.060	56.719	1.00	47.93	C
ATOM	2692	N	ARG	C	64	50.459	112.044	55.346	1.00	50.16	C
ATOM	2693	CA	ARG	C	64	51.576	111.286	55.873	1.00	50.16	C
ATOM	2694	CB	ARG	C	64	51.810	110.042	55.007	1.00	47.99	C
ATOM	2695	CG	ARG	C	64	50.556	109.303	54.600	1.00	47.99	C
ATOM	2696	CD	ARG	C	64	50.425	107.994	55.347	1.00	47.99	C
ATOM	2697	NE	ARG	C	64	49.260	107.231	54.901	1.00	47.99	C
ATOM	2698	CZ	ARG	C	64	47.998	107.552	55.171	1.00	47.99	C
ATOM	2699	NH1	ARG	C	64	47.716	108.628	55.901	1.00	47.99	C
ATOM	2700	NH2	ARG	C	64	47.014	106.799	54.695	1.00	47.99	C
ATOM	2701	C	ARG	C	64	52.851	112.100	55.867	1.00	50.16	C
ATOM	2702	O	ARG	C	64	52.871	113.251	55.446	1.00	50.16	C
ATOM	2703	N	GLN	C	65	53.909	111.465	56.360	1.00	41.79	C
ATOM	2704	CA	GLN	C	65	55.249	112.025	56.374	1.00	41.79	C
ATOM	2705	CB	GLN	C	65	55.822	112.089	57.792	1.00	50.64	C
ATOM	2706	CG	GLN	C	65	55.070	112.988	58.751	1.00	50.64	C
ATOM	2707	CD	GLN	C	65	55.856	113.264	60.030	1.00	50.64	C
ATOM	2708	OE1	GLN	C	65	56.883	113.951	60.007	1.00	50.64	C
ATOM	2709	NE2	GLN	C	65	55.378	112.723	61.151	1.00	50.64	C
ATOM	2710	C	GLN	C	65	56.017	110.979	55.566	1.00	41.79	C
ATOM	2711	O	GLN	C	65	55.709	109.788	55.638	1.00	41.79	C
ATOM	2712	N	LEU	C	66	56.987	111.410	54.773	1.00	42.83	C
ATOM	2713	CA	LEU	C	66	57.758	110.451	54.001	1.00	42.83	C
ATOM	2714	CB	LEU	C	66	57.852	110.855	52.531	1.00	44.65	C
ATOM	2715	CG	LEU	C	66	56.892	110.109	51.610	1.00	44.65	C
ATOM	2716	CD1	LEU	C	66	57.176	110.499	50.169	1.00	44.65	C
ATOM	2717	CD2	LEU	C	66	57.059	108.611	51.791	1.00	44.65	C
ATOM	2718	C	LEU	C	66	59.136	110.351	54.593	1.00	42.83	C
ATOM	2719	O	LEU	C	66	59.952	111.262	54.453	1.00	42.83	C
ATOM	2720	N	TYR	C	67	59.387	109.232	55.261	1.00	48.46	C
ATOM	2721	CA	TYR	C	67	60.671	109.007	55.896	1.00	48.46	C
ATOM	2722	CB	TYR	C	67	60.480	108.303	57.236	1.00	54.10	C

FIGURE 2 Continued

ATOM	2723	CG	TYR	C	67	61.774	108.057	57.971	1.00	54.10	C
ATOM	2724	CD1	TYR	C	67	62.508	109.115	58.507	1.00	54.10	C
ATOM	2725	CE1	TYR	C	67	63.705	108.886	59.184	1.00	54.10	C
ATOM	2726	CD2	TYR	C	67	62.272	106.762	58.128	1.00	54.10	C
ATOM	2727	CE2	TYR	C	67	63.461	106.524	58.799	1.00	54.10	C
ATOM	2728	CZ	TYR	C	67	64.172	107.586	59.325	1.00	54.10	C
ATOM	2729	OH	TYR	C	67	65.348	107.345	59.993	1.00	54.10	C
ATOM	2730	C	TYR	C	67	61.601	108.185	55.017	1.00	48.46	C
ATOM	2731	O	TYR	C	67	61.342	107.012	54.737	1.00	48.46	C
ATOM	2732	N	CYS	C	68	62.682	108.820	54.581	1.00	46.82	C
ATOM	2733	CA	CYS	C	68	63.669	108.164	53.748	1.00	46.82	C
ATOM	2734	CB	CYS	C	68	64.490	109.212	53.000	1.00	54.28	C
ATOM	2735	SG	CYS	C	68	65.590	108.523	51.757	1.00	54.28	C
ATOM	2736	C	CYS	C	68	64.567	107.343	54.673	1.00	46.82	C
ATOM	2737	O	CYS	C	68	64.946	107.817	55.751	1.00	46.82	C
ATOM	2738	N	ARG	C	69	64.898	106.120	54.259	1.00	54.93	C
ATOM	2739	CA	ARG	C	69	65.743	105.243	55.063	1.00	54.93	C
ATOM	2740	CB	ARG	C	69	66.038	103.940	54.311	1.00	96.31	C
ATOM	2741	CG	ARG	C	69	66.932	102.972	55.079	1.00	96.31	C
ATOM	2742	CD	ARG	C	69	66.313	102.550	56.409	1.00	96.31	C

FIGURE 2 Continued

ATOM	2743	NE	ARG	C	69	67.327	102.373	57.450	1.00	96.31	C
ATOM	2744	CZ	ARG	C	69	68.270	101.435	57.440	1.00	96.31	C
ATOM	2745	NH1	ARG	C	69	68.340	100.564	56.439	1.00	96.31	C
ATOM	2746	NH2	ARG	C	69	69.157	101.377	58.426	1.00	96.31	C
ATOM	2747	C	ARG	C	69	67.049	105.947	55.437	1.00	54.93	C
ATOM	2748	O	ARG	C	69	67.742	105.559	56.381	1.00	54.93	C
ATOM	2749	N	THR	C	70	67.363	106.998	54.694	1.00	49.77	C
ATOM	2750	CA	THR	C	70	68.564	107.784	54.926	1.00	49.77	C
ATOM	2751	CB	THR	C	70	68.787	108.765	53.752	1.00	63.59	C
ATOM	2752	OG1	THR	C	70	70.135	109.239	53.769	1.00	63.59	C
ATOM	2753	CG2	THR	C	70	67.840	109.950	53.859	1.00	63.59	C
ATOM	2754	C	THR	C	70	68.442	108.561	56.246	1.00	49.77	C
ATOM	2755	O	THR	C	70	69.415	109.139	56.728	1.00	49.77	C
ATOM	2756	N	GLY	C	71	67.239	108.576	56.821	1.00	51.51	C
ATOM	2757	CA	GLY	C	71	67.014	109.270	58.078	1.00	51.51	C
ATOM	2758	C	GLY	C	71	66.345	110.633	57.986	1.00	51.51	C
ATOM	2759	O	GLY	C	71	66.274	111.357	58.981	1.00	51.51	C
ATOM	2760	N	PHE	C	72	65.846	110.994	56.807	1.00	48.91	C
ATOM	2761	CA	PHE	C	72	65.201	112.295	56.642	1.00	48.91	C
ATOM	2762	CB	PHE	C	72	66.019	113.194	55.719	1.00	54.63	C
ATOM	2763	CG	PHE	C	72	67.404	113.459	56.198	1.00	54.63	C
ATOM	2764	CD1	PHE	C	72	68.395	112.496	56.066	1.00	54.63	C
ATOM	2765	CD2	PHE	C	72	67.722	114.679	56.782	1.00	54.63	C
ATOM	2766	CE1	PHE	C	72	69.688	112.748	56.508	1.00	54.63	C
ATOM	2767	CE2	PHE	C	72	69.007	114.940	57.226	1.00	54.63	C
ATOM	2768	CZ	PHE	C	72	69.993	113.975	57.090	1.00	54.63	C
ATOM	2769	C	PHE	C	72	63.793	112.245	56.083	1.00	48.91	C
ATOM	2770	O	PHE	C	72	63.442	111.351	55.314	1.00	48.91	C
ATOM	2771	N	HIS	C	73	62.991	113.229	56.469	1.00	42.55	C
ATOM	2772	CA	HIS	C	73	61.629	113.344	55.970	1.00	42.55	C
ATOM	2773	CB	HIS	C	73	60.682	113.880	57.045	1.00	45.15	C
ATOM	2774	CG	HIS	C	73	60.388	112.905	58.138	1.00	45.15	C
ATOM	2775	CD2	HIS	C	73	59.430	111.953	58.248	1.00	45.15	C
ATOM	2776	ND1	HIS	C	73	61.127	112.843	59.299	1.00	45.15	C
ATOM	2777	CE1	HIS	C	73	60.634	111.896	60.080	1.00	45.15	C
ATOM	2778	NE2	HIS	C	73	59.604	111.341	59.465	1.00	45.15	C
ATOM	2779	C	HIS	C	73	61.627	114.309	54.792	1.00	42.55	C
ATOM	2780	O	HIS	C	73	62.266	115.363	54.828	1.00	42.55	C
ATOM	2781	N	LEU	C	74	60.905	113.941	53.745	1.00	42.14	C
ATOM	2782	CA	LEU	C	74	60.812	114.783	52.569	1.00	42.14	C
ATOM	2783	CB	LEU	C	74	60.150	114.005	51.433	1.00	50.46	C
ATOM	2784	CG	LEU	C	74	60.181	114.628	50.038	1.00	50.46	C
ATOM	2785	CD1	LEU	C	74	61.586	114.549	49.482	1.00	50.46	C
ATOM	2786	CD2	LEU	C	74	59.231	113.876	49.128	1.00	50.46	C
ATOM	2787	C	LEU	C	74	59.986	116.028	52.897	1.00	42.14	C
ATOM	2788	O	LEU	C	74	58.870	115.928	53.415	1.00	42.14	C
ATOM	2789	N	GLU	C	75	60.546	117.199	52.606	1.00	42.02	C
ATOM	2790	CA	GLU	C	75	59.858	118.469	52.833	1.00	42.02	C
ATOM	2791	CB	GLU	C	75	60.686	119.388	53.728	1.00	61.65	C
ATOM	2792	CG	GLU	C	75	60.942	118.890	55.124	1.00	61.65	C
ATOM	2793	CD	GLU	C	75	61.856	119.824	55.884	1.00	61.65	C
ATOM	2794	OE1	GLU	C	75	63.080	119.799	55.629	1.00	61.65	C
ATOM	2795	OE2	GLU	C	75	61.346	120.597	56.724	1.00	61.65	C
ATOM	2796	C	GLU	C	75	59.639	119.188	51.505	1.00	42.02	C
ATOM	2797	O	GLU	C	75	60.546	119.260	50.680	1.00	42.02	C
ATOM	2798	N	ILE	C	76	58.440	119.714	51.295	1.00	41.08	C
ATOM	2799	CA	ILE	C	76	58.156	120.463	50.075	1.00	41.08	C

FIGURE 2 Continued

ATOM	2800	CB	ILE	C	76	56.900	119.918	49.358	1.00	31.52	C
ATOM	2801	CG2	ILE	C	76	56.571	120.796	48.150	1.00	31.52	C
ATOM	2802	CG1	ILE	C	76	57.136	118.454	48.954	1.00	31.52	C
ATOM	2803	CD1	ILE	C	76	55.946	117.758	48.325	1.00	31.52	C
ATOM	2804	C	ILE	C	76	57.951	121.927	50.490	1.00	41.08	C
ATOM	2805	O	ILE	C	76	56.954	122.282	51.122	1.00	41.08	C
ATOM	2806	N	PHE	C	77	58.918	122.769	50.149	1.00	46.90	C
ATOM	2807	CA	PHE	C	77	58.870	124.174	50.519	1.00	46.90	C
ATOM	2808	CB	PHE	C	77	60.296	124.712	50.660	1.00	43.12	C
ATOM	2809	CG	PHE	C	77	60.961	124.302	51.941	1.00	43.12	C
ATOM	2810	CD1	PHE	C	77	60.692	124.981	53.127	1.00	43.12	C
ATOM	2811	CD2	PHE	C	77	61.797	123.199	51.985	1.00	43.12	C
ATOM	2812	CE1	PHE	C	77	61.248	124.559	54.341	1.00	43.12	C
ATOM	2813	CE2	PHE	C	77	62.354	122.773	53.193	1.00	43.12	C
ATOM	2814	CZ	PHE	C	77	62.076	123.454	54.371	1.00	43.12	C
ATOM	2815	C	PHE	C	77	58.053	125.066	49.602	1.00	46.90	C
ATOM	2816	O	PHE	C	77	57.856	124.763	48.423	1.00	46.90	C
ATOM	2817	N	PRO	C	78	57.551	126.184	50.150	1.00	46.05	C
ATOM	2818	CD	PRO	C	78	57.618	126.564	51.574	1.00	34.87	C
ATOM	2819	CA	PRO	C	78	56.742	127.144	49.397	1.00	46.05	C
ATOM	2820	CB	PRO	C	78	56.491	128.251	50.415	1.00	34.87	C
ATOM	2821	CG	PRO	C	78	56.432	127.497	51.704	1.00	34.87	C
ATOM	2822	C	PRO	C	78	57.433	127.645	48.135	1.00	46.05	C
ATOM	2823	O	PRO	C	78	56.777	127.845	47.118	1.00	46.05	C
ATOM	2824	N	ASN	C	79	58.749	127.845	48.182	1.00	45.01	C
ATOM	2825	CA	ASN	C	79	59.449	128.313	46.991	1.00	45.01	C
ATOM	2826	CB	ASN	C	79	60.763	129.015	47.340	1.00	49.74	C
ATOM	2827	CG	ASN	C	79	61.668	128.189	48.225	1.00	49.74	C
ATOM	2828	OD1	ASN	C	79	61.667	126.951	48.180	1.00	49.74	C
ATOM	2829	ND2	ASN	C	79	62.467	128.906	49.015	1.00	49.74	C
ATOM	2830	C	ASN	C	79	59.723	127.199	45.989	1.00	45.01	C
ATOM	2831	O	ASN	C	79	60.527	127.363	45.071	1.00	45.01	C
ATOM	2832	N	GLY	C	80	59.055	126.064	46.167	1.00	47.67	C
ATOM	2833	CA	GLY	C	80	59.224	124.955	45.246	1.00	47.67	C
ATOM	2834	C	GLY	C	80	60.463	124.112	45.466	1.00	47.67	C
ATOM	2835	O	GLY	C	80	60.762	123.217	44.684	1.00	47.67	C
ATOM	2836	N	THR	C	81	61.189	124.396	46.532	1.00	40.35	C
ATOM	2837	CA	THR	C	81	62.389	123.644	46.838	1.00	40.35	C
ATOM	2838	CB	THR	C	81	63.383	124.535	47.605	1.00	62.47	C
ATOM	2839	OG1	THR	C	81	64.064	125.376	46.667	1.00	62.47	C
ATOM	2840	CG2	THR	C	81	64.398	123.706	48.367	1.00	62.47	C
ATOM	2841	C	THR	C	81	62.071	122.374	47.628	1.00	40.35	C
ATOM	2842	O	THR	C	81	61.089	122.310	48.368	1.00	40.35	C
ATOM	2843	N	ILE	C	82	62.894	121.352	47.429	1.00	48.55	C
ATOM	2844	CA	ILE	C	82	62.716	120.087	48.110	1.00	48.55	C
ATOM	2845	CB	ILE	C	82	62.677	118.909	47.114	1.00	35.35	C
ATOM	2846	CG2	ILE	C	82	62.562	117.573	47.876	1.00	35.35	C
ATOM	2847	CG1	ILE	C	82	61.498	119.098	46.164	1.00	35.35	C
ATOM	2848	CD1	ILE	C	82	60.195	119.305	46.886	1.00	35.35	C
ATOM	2849	C	ILE	C	82	63.880	119.929	49.055	1.00	48.55	C
ATOM	2850	O	ILE	C	82	65.009	120.269	48.714	1.00	48.55	C
ATOM	2851	N	GLN	C	83	63.606	119.393	50.237	1.00	39.36	C
ATOM	2852	CA	GLN	C	83	64.637	119.251	51.250	1.00	39.36	C
ATOM	2853	CB	GLN	C	83	64.698	120.564	52.035	1.00	65.22	C
ATOM	2854	CG	GLN	C	83	65.819	120.712	53.033	1.00	65.22	C
ATOM	2855	CD	GLN	C	83	65.788	122.080	53.696	1.00	65.22	C
ATOM	2856	OE1	GLN	C	83	65.959	123.108	53.033	1.00	65.22	C

FIGURE 2 Continued

ATOM	2857	NE2	GLN	C	83	65.552	122.099	55.007	1.00	65.22	C
ATOM	2858	C	GLN	C	83	64.326	118.083	52.180	1.00	39.36	C
ATOM	2859	O	GLN	C	83	63.247	117.505	52.122	1.00	39.36	C
ATOM	2860	N	GLY	C	84	65.287	117.741	53.029	1.00	46.73	C
ATOM	2861	CA	GLY	C	84	65.100	116.651	53.966	1.00	46.73	C
ATOM	2862	C	GLY	C	84	65.369	117.127	55.378	1.00	46.73	C
ATOM	2863	O	GLY	C	84	66.242	117.965	55.602	1.00	46.73	C
ATOM	2864	N	THR	C	85	64.615	116.603	56.335	1.00	48.67	C
ATOM	2865	CA	THR	C	85	64.795	116.993	57.723	1.00	48.67	C
ATOM	2866	CB	THR	C	85	63.795	118.083	58.129	1.00	59.68	C
ATOM	2867	OG1	THR	C	85	64.077	118.506	59.467	1.00	59.68	C
ATOM	2868	CG2	THR	C	85	62.369	117.548	58.063	1.00	59.68	C
ATOM	2869	C	THR	C	85	64.616	115.813	58.668	1.00	48.67	C
ATOM	2870	O	THR	C	85	63.725	114.979	58.479	1.00	48.67	C
ATOM	2871	N	ARG	C	86	65.467	115.747	59.687	1.00	47.24	C
ATOM	2872	CA	ARG	C	86	65.384	114.675	60.672	1.00	47.24	C
ATOM	2873	CB	ARG	C	86	66.672	114.609	61.488	1.00	80.07	C
ATOM	2874	CG	ARG	C	86	67.859	114.170	60.676	1.00	80.07	C
ATOM	2875	CD	ARG	C	86	69.132	114.159	61.493	1.00	80.07	C
ATOM	2876	NE	ARG	C	86	70.212	113.498	60.766	1.00	80.07	C
ATOM	2877	CZ	ARG	C	86	70.171	112.230	60.362	1.00	80.07	C
ATOM	2878	NH1	ARG	C	86	69.101	111.484	60.616	1.00	80.07	C
ATOM	2879	NH2	ARG	C	86	71.196	111.708	59.698	1.00	80.07	C
ATOM	2880	C	ARG	C	86	64.193	114.917	61.593	1.00	47.24	C
ATOM	2881	O	ARG	C	86	63.651	113.980	62.178	1.00	47.24	C
ATOM	2882	N	LYS	C	87	63.787	116.180	61.699	1.00	58.17	C
ATOM	2883	CA	LYS	C	87	62.668	116.577	62.542	1.00	58.17	C
ATOM	2884	CB	LYS	C	87	62.381	118.067	62.374	1.00	93.57	C
ATOM	2885	CG	LYS	C	87	63.603	118.960	62.453	1.00	93.57	C
ATOM	2886	CD	LYS	C	87	64.198	118.998	63.849	1.00	93.57	C
ATOM	2887	CE	LYS	C	87	65.421	119.911	63.891	1.00	93.57	C
ATOM	2888	NZ	LYS	C	87	65.104	121.301	63.450	1.00	93.57	C
ATOM	2889	C	LYS	C	87	61.411	115.797	62.192	1.00	58.17	C
ATOM	2890	O	LYS	C	87	61.208	115.409	61.041	1.00	58.17	C
ATOM	2891	N	ASP	C	88	60.571	115.572	63.197	1.00	49.56	C
ATOM	2892	CA	ASP	C	88	59.313	114.858	63.020	1.00	49.56	C
ATOM	2893	CB	ASP	C	88	59.094	113.882	64.175	1.00	53.79	C
ATOM	2894	CG	ASP	C	88	57.745	113.195	64.113	1.00	53.79	C
ATOM	2895	OD1	ASP	C	88	57.372	112.687	63.036	1.00	53.79	C
ATOM	2896	OD2	ASP	C	88	57.052	113.151	65.147	1.00	53.79	C
ATOM	2897	C	ASP	C	88	58.204	115.900	62.990	1.00	49.56	C
ATOM	2898	O	ASP	C	88	58.297	116.927	63.657	1.00	49.56	C
ATOM	2899	N	HIS	C	89	57.167	115.643	62.202	1.00	58.06	C
ATOM	2900	CA	HIS	C	89	56.043	116.567	62.082	1.00	58.06	C
ATOM	2901	CB	HIS	C	89	55.211	116.572	63.355	1.00	49.88	C
ATOM	2902	CG	HIS	C	89	54.337	115.375	63.484	1.00	49.88	C
ATOM	2903	CD2	HIS	C	89	53.215	115.019	62.815	1.00	49.88	C
ATOM	2904	ND1	HIS	C	89	54.626	114.335	64.338	1.00	49.88	C
ATOM	2905	CE1	HIS	C	89	53.718	113.387	64.187	1.00	49.88	C
ATOM	2906	NE2	HIS	C	89	52.850	113.777	63.269	1.00	49.88	C
ATOM	2907	C	HIS	C	89	56.451	117.985	61.757	1.00	58.06	C
ATOM	2908	O	HIS	C	89	55.820	118.946	62.199	1.00	58.06	C
ATOM	2909	N	SER	C	90	57.512	118.113	60.982	1.00	46.04	C
ATOM	2910	CA	SER	C	90	57.977	119.424	60.590	1.00	46.04	C
ATOM	2911	CB	SER	C	90	59.296	119.324	59.823	1.00	57.14	C
ATOM	2912	OG	SER	C	90	59.098	118.708	58.560	1.00	57.14	C
ATOM	2913	C	SER	C	90	56.930	120.014	59.669	1.00	46.04	C

FIGURE 2 Continued

ATOM	2914	O	SER	C	90	56.219	119.291	58.965	1.00	46.04	C
ATOM	2915	N	ARG	C	91	56.815	121.330	59.693	1.00	90.55	C
ATOM	2916	CA	ARG	C	91	55.893	121.995	58.803	1.00	90.55	C
ATOM	2917	CB	ARG	C	91	55.849	123.480	59.149	1.00	75.27	C
ATOM	2918	CG	ARG	C	91	54.928	124.318	58.306	1.00	75.27	C
ATOM	2919	CD	ARG	C	91	55.165	125.773	58.608	1.00	75.27	C
ATOM	2920	NE	ARG	C	91	54.482	126.638	57.658	1.00	75.27	C
ATOM	2921	CZ	ARG	C	91	54.871	127.877	57.372	1.00	75.27	C
ATOM	2922	NH1	ARG	C	91	55.942	128.391	57.967	1.00	75.27	C
ATOM	2923	NH2	ARG	C	91	54.196	128.598	56.486	1.00	75.27	C
ATOM	2924	C	ARG	C	91	56.620	121.757	57.482	1.00	90.55	C
ATOM	2925	O	ARG	C	91	57.855	121.804	57.444	1.00	90.55	C
ATOM	2926	N	PHE	C	92	55.877	121.467	56.419	1.00	56.17	C
ATOM	2927	CA	PHE	C	92	56.477	121.213	55.099	1.00	56.17	C
ATOM	2928	CB	PHE	C	92	57.716	122.087	54.868	1.00	56.97	C
ATOM	2929	CG	PHE	C	92	57.455	123.553	55.000	1.00	56.97	C
ATOM	2930	CD1	PHE	C	92	56.395	124.149	54.323	1.00	56.97	C
ATOM	2931	CD2	PHE	C	92	58.267	124.344	55.808	1.00	56.97	C
ATOM	2932	CE1	PHE	C	92	56.145	125.515	54.452	1.00	56.97	C
ATOM	2933	CE2	PHE	C	92	58.029	125.709	55.945	1.00	56.97	C
ATOM	2934	CZ	PHE	C	92	56.965	126.297	55.265	1.00	56.97	C
ATOM	2935	C	PHE	C	92	56.854	119.745	54.893	1.00	56.17	C
ATOM	2936	O	PHE	C	92	57.224	119.335	53.794	1.00	56.17	C
ATOM	2937	N	GLY	C	93	56.766	118.966	55.963	1.00	43.07	C
ATOM	2938	CA	GLY	C	93	57.063	117.551	55.888	1.00	43.07	C
ATOM	2939	C	GLY	C	93	55.739	116.812	55.967	1.00	43.07	C
ATOM	2940	O	GLY	C	93	55.693	115.578	55.919	1.00	43.07	C
ATOM	2941	N	ILE	C	94	54.659	117.583	56.107	1.00	48.14	C
ATOM	2942	CA	ILE	C	94	53.316	117.016	56.178	1.00	48.14	C
ATOM	2943	CB	ILE	C	94	52.361	117.901	57.022	1.00	37.80	C
ATOM	2944	CG2	ILE	C	94	50.990	117.247	57.123	1.00	37.80	C
ATOM	2945	CG1	ILE	C	94	52.957	118.120	58.414	1.00	37.80	C
ATOM	2946	CD1	ILE	C	94	53.383	116.831	59.125	1.00	37.80	C
ATOM	2947	C	ILE	C	94	52.834	116.951	54.737	1.00	48.14	C
ATOM	2948	O	ILE	C	94	52.651	117.979	54.081	1.00	48.14	C
ATOM	2949	N	LEU	C	95	52.628	115.732	54.256	1.00	40.90	C
ATOM	2950	CA	LEU	C	95	52.237	115.508	52.874	1.00	40.90	C
ATOM	2951	CB	LEU	C	95	53.327	114.697	52.168	1.00	37.62	C
ATOM	2952	CG	LEU	C	95	54.780	115.076	52.494	1.00	37.62	C
ATOM	2953	CD1	LEU	C	95	55.710	114.037	51.905	1.00	37.62	C
ATOM	2954	CD2	LEU	C	95	55.109	116.454	51.948	1.00	37.62	C
ATOM	2955	C	LEU	C	95	50.928	114.770	52.717	1.00	40.90	C
ATOM	2956	O	LEU	C	95	50.541	113.960	53.562	1.00	40.90	C
ATOM	2957	N	GLU	C	96	50.252	115.043	51.612	1.00	37.54	C
ATOM	2958	CA	GLU	C	96	49.004	114.364	51.319	1.00	37.54	C
ATOM	2959	CB	GLU	C	96	47.917	115.358	50.948	1.00	62.78	C
ATOM	2960	CG	GLU	C	96	46.558	114.725	50.819	1.00	62.78	C
ATOM	2961	CD	GLU	C	96	45.581	115.641	50.141	1.00	62.78	C
ATOM	2962	OE1	GLU	C	96	45.654	116.865	50.389	1.00	62.78	C
ATOM	2963	OE2	GLU	C	96	44.738	115.141	49.366	1.00	62.78	C
ATOM	2964	C	GLU	C	96	49.235	113.423	50.143	1.00	37.54	C
ATOM	2965	O	GLU	C	96	49.601	113.859	49.048	1.00	37.54	C
ATOM	2966	N	PHE	C	97	49.039	112.132	50.376	1.00	51.61	C
ATOM	2967	CA	PHE	C	97	49.200	111.158	49.315	1.00	51.61	C
ATOM	2968	CB	PHE	C	97	49.544	109.785	49.887	1.00	45.25	C
ATOM	2969	CG	PHE	C	97	51.010	109.574	50.078	1.00	45.25	C
ATOM	2970	CD1	PHE	C	97	51.762	110.467	50.838	1.00	45.25	C

FIGURE 2 Continued

ATOM	2971	CD2	PHE	C	97	51.651	108.498	49.481	1.00	45.25	C
ATOM	2972	CE1	PHE	C	97	53.135	110.290	50.998	1.00	45.25	C
ATOM	2973	CE2	PHE	C	97	53.026	108.311	49.635	1.00	45.25	C
ATOM	2974	CZ	PHE	C	97	53.769	109.208	50.393	1.00	45.25	C
ATOM	2975	C	PHE	C	97	47.921	111.086	48.512	1.00	51.61	C
ATOM	2976	O	PHE	C	97	46.849	110.831	49.048	1.00	51.61	C
ATOM	2977	N	ILE	C	98	48.036	111.338	47.220	1.00	47.54	C
ATOM	2978	CA	ILE	C	98	46.890	111.292	46.339	1.00	47.54	C
ATOM	2979	CB	ILE	C	98	46.865	112.521	45.432	1.00	47.84	C
ATOM	2980	CG2	ILE	C	98	45.652	112.479	44.520	1.00	47.84	C
ATOM	2981	CG1	ILE	C	98	46.857	113.778	46.289	1.00	47.84	C
ATOM	2982	CD1	ILE	C	98	46.992	115.031	45.488	1.00	47.84	C
ATOM	2983	C	ILE	C	98	47.017	110.037	45.487	1.00	47.54	C
ATOM	2984	O	ILE	C	98	48.048	109.816	44.846	1.00	47.54	C
ATOM	2985	N	SER	C	99	45.978	109.208	45.493	1.00	68.65	C
ATOM	2986	CA	SER	C	99	45.990	107.982	44.708	1.00	68.65	C
ATOM	2987	CB	SER	C	99	45.126	106.916	45.375	1.00	60.37	C
ATOM	2988	OG	SER	C	99	45.237	105.688	44.683	1.00	60.37	C
ATOM	2989	C	SER	C	99	45.484	108.266	43.296	1.00	68.65	C
ATOM	2990	O	SER	C	99	44.287	108.386	43.061	1.00	68.65	C
ATOM	2991	N	ILE	C	100	46.421	108.379	42.364	1.00	45.89	C
ATOM	2992	CA	ILE	C	100	46.128	108.660	40.967	1.00	45.89	C
ATOM	2993	CB	ILE	C	100	47.425	109.062	40.227	1.00	42.18	C
ATOM	2994	CG2	ILE	C	100	47.176	109.151	38.728	1.00	42.18	C
ATOM	2995	CG1	ILE	C	100	47.957	110.377	40.802	1.00	42.18	C
ATOM	2996	CD1	ILE	C	100	47.029	111.561	40.628	1.00	42.18	C
ATOM	2997	C	ILE	C	100	45.513	107.451	40.263	1.00	45.89	C
ATOM	2998	O	ILE	C	100	44.634	107.590	39.418	1.00	45.89	C
ATOM	2999	N	ALA	C	101	45.992	106.266	40.615	1.00	42.48	C
ATOM	3000	CA	ALA	C	101	45.506	105.037	40.020	1.00	42.48	C
ATOM	3001	CB	ALA	C	101	45.751	105.045	38.513	1.00	44.15	C
ATOM	3002	C	ALA	C	101	46.261	103.897	40.669	1.00	42.48	C
ATOM	3003	O	ALA	C	101	47.077	104.120	41.564	1.00	42.48	C
ATOM	3004	N	VAL	C	102	45.993	102.678	40.220	1.00	53.84	C
ATOM	3005	CA	VAL	C	102	46.660	101.508	40.775	1.00	53.84	C
ATOM	3006	CB	VAL	C	102	46.148	100.205	40.112	1.00	65.50	C
ATOM	3007	CG1	VAL	C	102	46.804	98.993	40.760	1.00	65.50	C
ATOM	3008	CG2	VAL	C	102	44.630	100.122	40.240	1.00	65.50	C
ATOM	3009	C	VAL	C	102	48.164	101.610	40.570	1.00	53.84	C
ATOM	3010	O	VAL	C	102	48.643	101.675	39.435	1.00	53.84	C
ATOM	3011	N	GLY	C	103	48.904	101.636	41.673	1.00	50.95	C
ATOM	3012	CA	GLY	C	103	50.353	101.719	41.590	1.00	50.95	C
ATOM	3013	C	GLY	C	103	50.918	103.112	41.369	1.00	50.95	C
ATOM	3014	O	GLY	C	103	52.134	103.286	41.361	1.00	50.95	C
ATOM	3015	N	LEU	C	104	50.045	104.102	41.203	1.00	47.50	C
ATOM	3016	CA	LEU	C	104	50.473	105.473	40.974	1.00	47.50	C
ATOM	3017	CB	LEU	C	104	49.950	105.969	39.624	1.00	41.41	C
ATOM	3018	CG	LEU	C	104	50.320	105.165	38.368	1.00	41.41	C
ATOM	3019	CD1	LEU	C	104	49.739	105.861	37.133	1.00	41.41	C
ATOM	3020	CD2	LEU	C	104	51.835	105.042	38.245	1.00	41.41	C
ATOM	3021	C	LEU	C	104	49.982	106.420	42.059	1.00	47.50	C
ATOM	3022	O	LEU	C	104	48.862	106.283	42.545	1.00	47.50	C
ATOM	3023	N	VAL	C	105	50.822	107.381	42.435	1.00	36.41	C
ATOM	3024	CA	VAL	C	105	50.447	108.380	43.434	1.00	36.41	C
ATOM	3025	CB	VAL	C	105	51.016	108.080	44.853	1.00	35.73	C
ATOM	3026	CG1	VAL	C	105	50.599	106.702	45.323	1.00	35.73	C
ATOM	3027	CG2	VAL	C	105	52.536	108.228	44.839	1.00	35.73	C

FIGURE 2 Continued

ATOM	3028	C	VAL	C	105	50.983	109.757	43.081	1.00	36.41	C
ATOM	3029	O	VAL	C	105	51.826	109.919	42.197	1.00	36.41	C
ATOM	3030	N	SER	C	106	50.466	110.747	43.795	1.00	38.37	C
ATOM	3031	CA	SER	C	106	50.913	112.117	43.675	1.00	38.37	C
ATOM	3032	CB	SER	C	106	49.866	112.985	42.987	1.00	46.65	C
ATOM	3033	OG	SER	C	106	49.983	112.877	41.579	1.00	46.65	C
ATOM	3034	C	SER	C	106	51.106	112.526	45.138	1.00	38.37	C
ATOM	3035	O	SER	C	106	50.397	112.036	46.024	1.00	38.37	C
ATOM	3036	N	ILE	C	107	52.086	113.386	45.402	1.00	38.47	C
ATOM	3037	CA	ILE	C	107	52.354	113.808	46.769	1.00	38.47	C
ATOM	3038	CB	ILE	C	107	53.748	113.341	47.203	1.00	37.99	C
ATOM	3039	CG2	ILE	C	107	53.990	113.695	48.658	1.00	37.99	C
ATOM	3040	CG1	ILE	C	107	53.854	111.827	46.994	1.00	37.99	C
ATOM	3041	CD1	ILE	C	107	55.262	111.262	47.188	1.00	37.99	C
ATOM	3042	C	ILE	C	107	52.245	115.316	46.907	1.00	38.47	C
ATOM	3043	O	ILE	C	107	52.987	116.061	46.271	1.00	38.47	C
ATOM	3044	N	ARG	C	108	51.312	115.764	47.741	1.00	39.32	C
ATOM	3045	CA	ARG	C	108	51.113	117.195	47.932	1.00	39.32	C
ATOM	3046	CB	ARG	C	108	49.660	117.570	47.641	1.00	71.06	C
ATOM	3047	CG	ARG	C	108	49.439	119.069	47.577	1.00	71.06	C
ATOM	3048	CD	ARG	C	108	48.032	119.422	47.139	1.00	71.06	C
ATOM	3049	NE	ARG	C	108	47.937	120.833	46.779	1.00	71.06	C
ATOM	3050	CZ	ARG	C	108	46.838	121.415	46.310	1.00	71.06	C
ATOM	3051	NH1	ARG	C	108	45.728	120.706	46.145	1.00	71.06	C
ATOM	3052	NH2	ARG	C	108	46.850	122.705	45.999	1.00	71.06	C
ATOM	3053	C	ARG	C	108	51.497	117.713	49.316	1.00	39.32	C
ATOM	3054	O	ARG	C	108	50.983	117.242	50.331	1.00	39.32	C
ATOM	3055	N	GLY	C	109	52.418	118.672	49.351	1.00	47.30	C
ATOM	3056	CA	GLY	C	109	52.810	119.254	50.621	1.00	47.30	C
ATOM	3057	C	GLY	C	109	51.585	120.004	51.112	1.00	47.30	C
ATOM	3058	O	GLY	C	109	51.084	120.891	50.423	1.00	47.30	C
ATOM	3059	N	VAL	C	110	51.079	119.640	52.284	1.00	51.39	C
ATOM	3060	CA	VAL	C	110	49.883	120.285	52.816	1.00	51.39	C
ATOM	3061	CB	VAL	C	110	49.451	119.641	54.149	1.00	45.60	C
ATOM	3062	CG1	VAL	C	110	48.334	120.457	54.784	1.00	45.60	C
ATOM	3063	CG2	VAL	C	110	48.984	118.212	53.898	1.00	45.60	C
ATOM	3064	C	VAL	C	110	50.049	121.785	53.024	1.00	51.39	C
ATOM	3065	O	VAL	C	110	49.206	122.576	52.602	1.00	51.39	C
ATOM	3066	N	ASP	C	111	51.142	122.168	53.672	1.00	51.41	C
ATOM	3067	CA	ASP	C	111	51.408	123.567	53.942	1.00	51.41	C
ATOM	3068	CB	ASP	C	111	52.613	123.690	54.871	1.00	79.49	C
ATOM	3069	CG	ASP	C	111	52.703	125.046	55.524	1.00	79.49	C
ATOM	3070	OD1	ASP	C	111	52.976	126.029	54.805	1.00	79.49	C
ATOM	3071	OD2	ASP	C	111	52.492	125.128	56.754	1.00	79.49	C
ATOM	3072	C	ASP	C	111	51.642	124.360	52.656	1.00	51.41	C
ATOM	3073	O	ASP	C	111	50.904	125.297	52.365	1.00	51.41	C
ATOM	3074	N	SER	C	112	52.655	123.980	51.883	1.00	45.97	C
ATOM	3075	CA	SER	C	112	52.968	124.680	50.638	1.00	45.97	C
ATOM	3076	CB	SER	C	112	54.268	124.149	50.036	1.00	47.62	C
ATOM	3077	OG	SER	C	112	54.058	122.896	49.403	1.00	47.62	C
ATOM	3078	C	SER	C	112	51.869	124.544	49.591	1.00	45.97	C
ATOM	3079	O	SER	C	112	51.645	125.451	48.792	1.00	45.97	C
ATOM	3080	N	GLY	C	113	51.189	123.404	49.592	1.00	48.43	C
ATOM	3081	CA	GLY	C	113	50.148	123.177	48.614	1.00	48.43	C
ATOM	3082	C	GLY	C	113	50.771	122.794	47.284	1.00	48.43	C
ATOM	3083	O	GLY	C	113	50.075	122.690	46.271	1.00	48.43	C
ATOM	3084	N	LEU	C	114	52.083	122.575	47.280	1.00	50.49	C

FIGURE 2 Continued

ATOM	3085	CA	LEU	C	114	52.775	122.218	46.049	1.00	50.49	C
ATOM	3086	CB	LEU	C	114	54.153	122.889	46.001	1.00	42.01	C
ATOM	3087	CG	LEU	C	114	54.179	124.422	46.069	1.00	42.01	C
ATOM	3088	CD1	LEU	C	114	55.622	124.900	46.140	1.00	42.01	C
ATOM	3089	CD2	LEU	C	114	53.473	125.016	44.857	1.00	42.01	C
ATOM	3090	C	LEU	C	114	52.925	120.709	45.877	1.00	50.49	C
ATOM	3091	O	LEU	C	114	53.099	119.966	46.848	1.00	50.49	C
ATOM	3092	N	TYR	C	115	52.852	120.265	44.627	1.00	38.22	C
ATOM	3093	CA	TYR	C	115	52.979	118.849	44.305	1.00	38.22	C
ATOM	3094	CB	TYR	C	115	52.156	118.512	43.060	1.00	51.09	C
ATOM	3095	CG	TYR	C	115	50.673	118.714	43.231	1.00	51.09	C
ATOM	3096	CD1	TYR	C	115	49.875	117.735	43.819	1.00	51.09	C
ATOM	3097	CE1	TYR	C	115	48.500	117.921	43.968	1.00	51.09	C
ATOM	3098	CD2	TYR	C	115	50.062	119.890	42.798	1.00	51.09	C
ATOM	3099	CE2	TYR	C	115	48.700	120.089	42.941	1.00	51.09	C
ATOM	3100	CZ	TYR	C	115	47.922	119.105	43.523	1.00	51.09	C
ATOM	3101	OH	TYR	C	115	46.567	119.312	43.643	1.00	51.09	C
ATOM	3102	C	TYR	C	115	54.427	118.468	44.051	1.00	38.22	C
ATOM	3103	O	TYR	C	115	55.189	119.237	43.481	1.00	38.22	C
ATOM	3104	N	LEU	C	116	54.804	117.276	44.488	1.00	35.89	C
ATOM	3105	CA	LEU	C	116	56.148	116.796	44.265	1.00	35.89	C
ATOM	3106	CB	LEU	C	116	56.409	115.528	45.067	1.00	39.96	C
ATOM	3107	CG	LEU	C	116	57.839	115.007	44.919	1.00	39.96	C
ATOM	3108	CD1	LEU	C	116	58.791	116.004	45.549	1.00	39.96	C
ATOM	3109	CD2	LEU	C	116	57.976	113.645	45.586	1.00	39.96	C
ATOM	3110	C	LEU	C	116	56.230	116.473	42.781	1.00	35.89	C
ATOM	3111	O	LEU	C	116	55.378	115.748	42.235	1.00	35.89	C
ATOM	3112	N	GLY	C	117	57.244	117.016	42.121	1.00	33.68	C
ATOM	3113	CA	GLY	C	117	57.397	116.748	40.710	1.00	33.68	C
ATOM	3114	C	GLY	C	117	58.821	116.374	40.387	1.00	33.68	C
ATOM	3115	O	GLY	C	117	59.726	116.635	41.181	1.00	33.68	C
ATOM	3116	N	MET	C	118	59.025	115.727	39.245	1.00	38.46	C
ATOM	3117	CA	MET	C	118	60.375	115.386	38.823	1.00	38.46	C
ATOM	3118	CB	MET	C	118	60.690	113.908	39.021	1.00	34.68	C
ATOM	3119	CG	MET	C	118	62.165	113.655	38.798	1.00	34.68	C
ATOM	3120	SD	MET	C	118	62.632	111.942	38.667	1.00	34.68	C
ATOM	3121	CE	MET	C	118	62.965	111.531	40.409	1.00	34.68	C
ATOM	3122	C	MET	C	118	60.529	115.749	37.352	1.00	38.46	C
ATOM	3123	O	MET	C	118	59.799	115.242	36.497	1.00	38.46	C
ATOM	3124	N	ASN	C	119	61.478	116.633	37.059	1.00	41.83	C
ATOM	3125	CA	ASN	C	119	61.679	117.065	35.686	1.00	41.83	C
ATOM	3126	CB	ASN	C	119	62.261	118.485	35.649	1.00	35.45	C
ATOM	3127	CG	ASN	C	119	63.685	118.564	36.194	1.00	35.45	C
ATOM	3128	OD1	ASN	C	119	64.397	117.551	36.293	1.00	35.45	C
ATOM	3129	ND2	ASN	C	119	64.116	119.784	36.532	1.00	35.45	C
ATOM	3130	C	ASN	C	119	62.535	116.122	34.843	1.00	41.83	C
ATOM	3131	O	ASN	C	119	63.059	115.120	35.342	1.00	41.83	C
ATOM	3132	N	GLU	C	120	62.637	116.458	33.556	1.00	46.89	C
ATOM	3133	CA	GLU	C	120	63.394	115.708	32.559	1.00	46.89	C
ATOM	3134	CB	GLU	C	120	63.540	116.575	31.302	1.00	87.11	C
ATOM	3135	CG	GLU	C	120	64.328	115.965	30.148	1.00	87.11	C
ATOM	3136	CD	GLU	C	120	63.459	115.182	29.174	1.00	87.11	C
ATOM	3137	OE1	GLU	C	120	62.364	115.673	28.826	1.00	87.11	C
ATOM	3138	OE2	GLU	C	120	63.880	114.085	28.740	1.00	87.11	C
ATOM	3139	C	GLU	C	120	64.775	115.285	33.071	1.00	46.89	C
ATOM	3140	O	GLU	C	120	65.247	114.198	32.740	1.00	46.89	C
ATOM	3141	N	LYS	C	121	65.410	116.135	33.882	1.00	45.70	C

FIGURE 2 Continued

ATOM	3142	CA	LYS	C	121	66.743	115.855	34.423	1.00	45.70	C
ATOM	3143	CB	LYS	C	121	67.534	117.150	34.609	1.00	56.55	C
ATOM	3144	CG	LYS	C	121	67.560	118.084	33.415	1.00	56.55	C
ATOM	3145	CD	LYS	C	121	68.486	119.260	33.705	1.00	56.55	C
ATOM	3146	CE	LYS	C	121	68.118	120.503	32.904	1.00	56.55	C
ATOM	3147	NZ	LYS	C	121	66.794	121.077	33.307	1.00	56.55	C
ATOM	3148	C	LYS	C	121	66.733	115.112	35.755	1.00	45.70	C
ATOM	3149	O	LYS	C	121	67.775	114.977	36.406	1.00	45.70	C
ATOM	3150	N	GLY	C	122	65.561	114.642	36.171	1.00	45.28	C
ATOM	3151	CA	GLY	C	122	65.471	113.916	37.426	1.00	45.28	C
ATOM	3152	C	GLY	C	122	65.529	114.813	38.649	1.00	45.28	C
ATOM	3153	O	GLY	C	122	65.806	114.350	39.758	1.00	45.28	C
ATOM	3154	N	GLU	C	123	65.265	116.099	38.452	1.00	35.23	C
ATOM	3155	CA	GLU	C	123	65.294	117.040	39.567	1.00	35.23	C
ATOM	3156	CB	GLU	C	123	65.680	118.438	39.075	1.00	55.65	C
ATOM	3157	CG	GLU	C	123	67.082	118.563	38.523	1.00	55.65	C
ATOM	3158	CD	GLU	C	123	67.393	119.981	38.092	1.00	55.65	C
ATOM	3159	OE1	GLU	C	123	66.711	120.469	37.163	1.00	55.65	C
ATOM	3160	OE2	GLU	C	123	68.306	120.607	38.685	1.00	55.65	C
ATOM	3161	C	GLU	C	123	63.938	117.124	40.271	1.00	35.23	C
ATOM	3162	O	GLU	C	123	62.903	117.316	39.613	1.00	35.23	C
ATOM	3163	N	LEU	C	124	63.947	116.989	41.598	1.00	37.52	C
ATOM	3164	CA	LEU	C	124	62.709	117.089	42.371	1.00	37.52	C
ATOM	3165	CB	LEU	C	124	62.872	116.504	43.784	1.00	27.36	C
ATOM	3166	CG	LEU	C	124	63.221	115.019	43.885	1.00	27.36	C
ATOM	3167	CD1	LEU	C	124	63.456	114.655	45.335	1.00	27.36	C
ATOM	3168	CD2	LEU	C	124	62.098	114.183	43.263	1.00	27.36	C
ATOM	3169	C	LEU	C	124	62.352	118.561	42.503	1.00	37.52	C
ATOM	3170	O	LEU	C	124	63.231	119.417	42.516	1.00	37.52	C
ATOM	3171	N	TYR	C	125	61.063	118.851	42.598	1.00	43.13	C
ATOM	3172	CA	TYR	C	125	60.620	120.221	42.764	1.00	43.13	C
ATOM	3173	CB	TYR	C	125	60.807	121.017	41.466	1.00	39.47	C
ATOM	3174	CG	TYR	C	125	59.862	120.627	40.354	1.00	39.47	C
ATOM	3175	CD1	TYR	C	125	60.105	119.499	39.564	1.00	39.47	C
ATOM	3176	CE1	TYR	C	125	59.213	119.117	38.564	1.00	39.47	C
ATOM	3177	CD2	TYR	C	125	58.705	121.363	40.117	1.00	39.47	C
ATOM	3178	CE2	TYR	C	125	57.806	120.993	39.130	1.00	39.47	C
ATOM	3179	CZ	TYR	C	125	58.062	119.869	38.354	1.00	39.47	C
ATOM	3180	OH	TYR	C	125	57.153	119.498	37.380	1.00	39.47	C
ATOM	3181	C	TYR	C	125	59.154	120.237	43.177	1.00	43.13	C
ATOM	3182	O	TYR	C	125	58.437	119.259	42.970	1.00	43.13	C
ATOM	3183	N	GLY	C	126	58.725	121.345	43.780	1.00	35.54	C
ATOM	3184	CA	GLY	C	126	57.344	121.491	44.193	1.00	35.54	C
ATOM	3185	C	GLY	C	126	56.623	122.131	43.032	1.00	35.54	C
ATOM	3186	O	GLY	C	126	57.012	123.193	42.568	1.00	35.54	C
ATOM	3187	N	SER	C	127	55.571	121.484	42.558	1.00	46.20	C
ATOM	3188	CA	SER	C	127	54.811	121.980	41.422	1.00	46.20	C
ATOM	3189	CB	SER	C	127	54.608	120.827	40.435	1.00	43.03	C
ATOM	3190	OG	SER	C	127	53.761	121.188	39.364	1.00	43.03	C
ATOM	3191	C	SER	C	127	53.462	122.581	41.839	1.00	46.20	C
ATOM	3192	O	SER	C	127	52.731	122.004	42.652	1.00	46.20	C
ATOM	3193	N	GLU	C	128	53.137	123.744	41.282	1.00	59.57	C
ATOM	3194	CA	GLU	C	128	51.879	124.406	41.597	1.00	59.57	C
ATOM	3195	CB	GLU	C	128	51.820	125.785	40.946	1.00	93.76	C
ATOM	3196	CG	GLU	C	128	52.544	126.866	41.714	1.00	93.76	C
ATOM	3197	CD	GLU	C	128	52.290	128.248	41.139	1.00	93.76	C
ATOM	3198	OE1	GLU	C	128	51.103	128.605	40.950	1.00	93.76	C

FIGURE 2 Continued

ATOM	3199	OE2	GLU	C	128	53.275	128.978	40.883	1.00	93.76	C
ATOM	3200	C	GLU	C	128	50.690	123.577	41.132	1.00	59.57	C
ATOM	3201	O	GLU	C	128	49.720	123.394	41.868	1.00	59.57	C
ATOM	3202	N	LYS	C	129	50.769	123.077	39.904	1.00	49.47	C
ATOM	3203	CA	LYS	C	129	49.697	122.268	39.345	1.00	49.47	C
ATOM	3204	CB	LYS	C	129	49.317	122.792	37.958	1.00	99.12	C
ATOM	3205	CG	LYS	C	129	48.730	124.194	37.984	1.00	99.12	C
ATOM	3206	CD	LYS	C	129	48.259	124.639	36.608	1.00	99.12	C
ATOM	3207	CE	LYS	C	129	47.640	126.034	36.661	1.00	99.12	C
ATOM	3208	NZ	LYS	C	129	47.140	126.488	35.329	1.00	99.12	C
ATOM	3209	C	LYS	C	129	50.068	120.789	39.260	1.00	49.47	C
ATOM	3210	O	LYS	C	129	51.244	120.419	39.266	1.00	49.47	C
ATOM	3211	N	LEU	C	130	49.050	119.946	39.188	1.00	60.11	C
ATOM	3212	CA	LEU	C	130	49.265	118.517	39.094	1.00	60.11	C
ATOM	3213	CB	LEU	C	130	48.028	117.763	39.584	1.00	52.06	C
ATOM	3214	CG	LEU	C	130	48.148	116.241	39.669	1.00	52.06	C
ATOM	3215	CD1	LEU	C	130	49.190	115.871	40.699	1.00	52.06	C
ATOM	3216	CD2	LEU	C	130	46.804	115.652	40.052	1.00	52.06	C
ATOM	3217	C	LEU	C	130	49.531	118.172	37.639	1.00	60.11	C
ATOM	3218	O	LEU	C	130	48.632	118.245	36.811	1.00	60.11	C
ATOM	3219	N	THR	C	131	50.765	117.802	37.324	1.00	39.89	C
ATOM	3220	CA	THR	C	131	51.115	117.452	35.955	1.00	39.89	C
ATOM	3221	CB	THR	C	131	52.198	118.389	35.399	1.00	44.42	C
ATOM	3222	OG1	THR	C	131	53.430	118.166	36.100	1.00	44.42	C
ATOM	3223	CG2	THR	C	131	51.772	119.845	35.572	1.00	44.42	C
ATOM	3224	C	THR	C	131	51.636	116.028	35.900	1.00	39.89	C
ATOM	3225	O	THR	C	131	51.732	115.350	36.924	1.00	39.89	C
ATOM	3226	N	GLN	C	132	51.969	115.569	34.702	1.00	46.49	C
ATOM	3227	CA	GLN	C	132	52.488	114.220	34.545	1.00	46.49	C
ATOM	3228	CB	GLN	C	132	52.669	113.906	33.067	1.00	55.46	C
ATOM	3229	CG	GLN	C	132	51.365	113.607	32.367	1.00	55.46	C
ATOM	3230	CD	GLN	C	132	51.522	113.510	30.870	1.00	55.46	C
ATOM	3231	OE1	GLN	C	132	52.541	113.033	30.382	1.00	55.46	C
ATOM	3232	NE2	GLN	C	132	50.506	113.950	30.129	1.00	55.46	C
ATOM	3233	C	GLN	C	132	53.800	114.040	35.302	1.00	46.49	C
ATOM	3234	O	GLN	C	132	54.164	112.921	35.656	1.00	46.49	C
ATOM	3235	N	GLU	C	133	54.497	115.144	35.566	1.00	41.72	C
ATOM	3236	CA	GLU	C	133	55.765	115.082	36.294	1.00	41.72	C
ATOM	3237	CB	GLU	C	133	56.607	116.334	36.039	1.00	47.86	C
ATOM	3238	CG	GLU	C	133	56.918	116.622	34.588	1.00	47.86	C
ATOM	3239	CD	GLU	C	133	58.126	117.534	34.430	1.00	47.86	C
ATOM	3240	OE1	GLU	C	133	58.312	118.442	35.271	1.00	47.86	C
ATOM	3241	OE2	GLU	C	133	58.890	117.349	33.459	1.00	47.86	C
ATOM	3242	C	GLU	C	133	55.534	114.940	37.799	1.00	41.72	C
ATOM	3243	O	GLU	C	133	56.487	114.903	38.581	1.00	41.72	C
ATOM	3244	N	CYS	C	134	54.264	114.855	38.194	1.00	41.75	C
ATOM	3245	CA	CYS	C	134	53.898	114.720	39.602	1.00	41.75	C
ATOM	3246	CB	CYS	C	134	52.918	115.828	39.986	1.00	38.75	C
ATOM	3247	SG	CYS	C	134	53.502	117.458	39.551	1.00	38.75	C
ATOM	3248	C	CYS	C	134	53.273	113.362	39.922	1.00	41.75	C
ATOM	3249	O	CYS	C	134	52.767	113.145	41.021	1.00	41.75	C
ATOM	3250	N	VAL	C	135	53.302	112.456	38.954	1.00	40.65	C
ATOM	3251	CA	VAL	C	135	52.733	111.130	39.139	1.00	40.65	C
ATOM	3252	CB	VAL	C	135	51.840	110.751	37.939	1.00	28.55	C
ATOM	3253	CG1	VAL	C	135	51.197	109.396	38.165	1.00	28.55	C
ATOM	3254	CG2	VAL	C	135	50.766	111.822	37.746	1.00	28.55	C
ATOM	3255	C	VAL	C	135	53.875	110.141	39.293	1.00	40.65	C

FIGURE 2 Continued

ATOM	3256	O	VAL	C	135	54.719	110.015	38.419	1.00	40.65	C
ATOM	3257	N	PHE	C	136	53.902	109.444	40.419	1.00	42.01	C
ATOM	3258	CA	PHE	C	136	54.974	108.504	40.697	1.00	42.01	C
ATOM	3259	CB	PHE	C	136	55.696	108.917	41.984	1.00	39.60	C
ATOM	3260	CG	PHE	C	136	56.400	110.234	41.885	1.00	39.60	C
ATOM	3261	CD1	PHE	C	136	57.717	110.300	41.439	1.00	39.60	C
ATOM	3262	CD2	PHE	C	136	55.736	111.414	42.203	1.00	39.60	C
ATOM	3263	CE1	PHE	C	136	58.368	111.534	41.315	1.00	39.60	C
ATOM	3264	CE2	PHE	C	136	56.375	112.650	42.081	1.00	39.60	C
ATOM	3265	CZ	PHE	C	136	57.696	112.712	41.635	1.00	39.60	C
ATOM	3266	C	PHE	C	136	54.522	107.067	40.838	1.00	42.01	C
ATOM	3267	O	PHE	C	136	53.387	106.783	41.226	1.00	42.01	C
ATOM	3268	N	ARG	C	137	55.435	106.160	40.524	1.00	40.27	C
ATOM	3269	CA	ARG	C	137	55.167	104.742	40.643	1.00	40.27	C
ATOM	3270	CB	ARG	C	137	56.026	103.948	39.666	1.00	54.39	C
ATOM	3271	CG	ARG	C	137	55.779	104.298	38.226	1.00	54.39	C
ATOM	3272	CD	ARG	C	137	56.588	103.397	37.325	1.00	54.39	C
ATOM	3273	NE	ARG	C	137	56.189	103.549	35.930	1.00	54.39	C
ATOM	3274	CZ	ARG	C	137	56.601	102.757	34.947	1.00	54.39	C
ATOM	3275	NH1	ARG	C	137	57.430	101.749	35.203	1.00	54.39	C
ATOM	3276	NH2	ARG	C	137	56.176	102.975	33.709	1.00	54.39	C
ATOM	3277	C	ARG	C	137	55.550	104.368	42.054	1.00	40.27	C
ATOM	3278	O	ARG	C	137	56.718	104.475	42.430	1.00	40.27	C
ATOM	3279	N	GLU	C	138	54.566	103.954	42.841	1.00	50.01	C
ATOM	3280	CA	GLU	C	138	54.812	103.547	44.222	1.00	50.01	C
ATOM	3281	CB	GLU	C	138	53.698	104.067	45.131	1.00	51.01	C
ATOM	3282	CG	GLU	C	138	53.764	103.577	46.564	1.00	51.01	C
ATOM	3283	CD	GLU	C	138	52.630	104.140	47.408	1.00	51.01	C
ATOM	3284	OE1	GLU	C	138	51.460	103.892	47.055	1.00	51.01	C
ATOM	3285	OE2	GLU	C	138	52.899	104.834	48.414	1.00	51.01	C
ATOM	3286	C	GLU	C	138	54.849	102.028	44.252	1.00	50.01	C
ATOM	3287	O	GLU	C	138	53.891	101.371	43.871	1.00	50.01	C
ATOM	3288	N	GLN	C	139	55.964	101.466	44.684	1.00	48.38	C
ATOM	3289	CA	GLN	C	139	56.074	100.018	44.732	1.00	48.38	C
ATOM	3290	CB	GLN	C	139	56.854	99.516	43.524	1.00	41.67	C
ATOM	3291	CG	GLN	C	139	56.224	99.881	42.190	1.00	41.67	C
ATOM	3292	CD	GLN	C	139	57.148	99.561	41.040	1.00	41.67	C
ATOM	3293	OE1	GLN	C	139	58.258	99.047	41.250	1.00	41.67	C
ATOM	3294	NE2	GLN	C	139	56.708	99.857	39.818	1.00	41.67	C
ATOM	3295	C	GLN	C	139	56.764	99.592	46.004	1.00	48.38	C
ATOM	3296	O	GLN	C	139	57.718	100.235	46.438	1.00	48.38	C
ATOM	3297	N	PHE	C	140	56.279	98.506	46.600	1.00	56.42	C
ATOM	3298	CA	PHE	C	140	56.853	98.012	47.843	1.00	56.42	C
ATOM	3299	CB	PHE	C	140	56.128	96.758	48.319	1.00	75.58	C
ATOM	3300	CG	PHE	C	140	56.599	96.272	49.657	1.00	75.58	C
ATOM	3301	CD1	PHE	C	140	56.033	96.763	50.828	1.00	75.58	C
ATOM	3302	CD2	PHE	C	140	57.637	95.348	49.750	1.00	75.58	C
ATOM	3303	CE1	PHE	C	140	56.494	96.339	52.072	1.00	75.58	C
ATOM	3304	CE2	PHE	C	140	58.104	94.923	50.989	1.00	75.58	C
ATOM	3305	CZ	PHE	C	140	57.532	95.418	52.151	1.00	75.58	C
ATOM	3306	C	PHE	C	140	58.330	97.690	47.694	1.00	56.42	C
ATOM	3307	O	PHE	C	140	58.776	97.252	46.635	1.00	56.42	C
ATOM	3308	N	GLU	C	141	59.082	97.895	48.766	1.00	71.76	C
ATOM	3309	CA	GLU	C	141	60.502	97.616	48.736	1.00	71.76	C
ATOM	3310	CB	GLU	C	141	61.290	98.924	48.684	1.00	58.43	C
ATOM	3311	CG	GLU	C	141	62.814	98.771	48.681	1.00	58.43	C
ATOM	3312	CD	GLU	C	141	63.351	98.081	47.435	1.00	58.43	C

FIGURE 2 Continued

ATOM	3313	OE1	GLU	C	141	62.738	98.225	46.353	1.00	58.43	C
ATOM	3314	OE2	GLU	C	141	64.401	97.406	47.535	1.00	58.43	C
ATOM	3315	C	GLU	C	141	60.960	96.792	49.931	1.00	71.76	C
ATOM	3316	O	GLU	C	141	61.148	95.583	49.819	1.00	71.76	C
ATOM	3317	N	GLU	C	142	61.119	97.443	51.079	1.00	88.30	C
ATOM	3318	CA	GLU	C	142	61.610	96.771	52.276	1.00	88.30	C
ATOM	3319	CB	GLU	C	142	63.128	97.005	52.366	1.00	89.84	C
ATOM	3320	CG	GLU	C	142	63.762	96.885	53.753	1.00	89.84	C
ATOM	3321	CD	GLU	C	142	64.235	98.229	54.316	1.00	89.84	C
ATOM	3322	OE1	GLU	C	142	64.832	99.030	53.560	1.00	89.84	C
ATOM	3323	OE2	GLU	C	142	64.023	98.477	55.522	1.00	89.84	C
ATOM	3324	C	GLU	C	142	60.930	97.196	53.576	1.00	88.30	C
ATOM	3325	O	GLU	C	142	60.989	98.360	53.964	1.00	88.30	C
ATOM	3326	N	ASN	C	143	60.288	96.240	54.242	1.00	62.50	C
ATOM	3327	CA	ASN	C	143	59.619	96.485	55.519	1.00	62.50	C
ATOM	3328	CB	ASN	C	143	60.656	96.683	56.625	1.00	82.91	C
ATOM	3329	CG	ASN	C	143	61.461	95.431	56.896	1.00	82.91	C
ATOM	3330	OD1	ASN	C	143	60.933	94.442	57.399	1.00	82.91	C
ATOM	3331	ND2	ASN	C	143	62.746	95.464	56.555	1.00	82.91	C
ATOM	3332	C	ASN	C	143	58.681	97.679	55.499	1.00	62.50	C
ATOM	3333	O	ASN	C	143	58.748	98.552	56.370	1.00	62.50	C
ATOM	3334	N	TRP	C	144	57.806	97.705	54.500	1.00	57.36	C
ATOM	3335	CA	TRP	C	144	56.824	98.765	54.334	1.00	57.36	C
ATOM	3336	CB	TRP	C	144	56.110	99.002	55.660	1.00	49.59	C
ATOM	3337	CG	TRP	C	144	55.271	97.819	55.972	1.00	49.59	C
ATOM	3338	CD2	TRP	C	144	54.223	97.294	55.153	1.00	49.59	C
ATOM	3339	CE2	TRP	C	144	53.766	96.110	55.768	1.00	49.59	C
ATOM	3340	CE3	TRP	C	144	53.631	97.709	53.953	1.00	49.59	C
ATOM	3341	CD1	TRP	C	144	55.400	96.963	57.030	1.00	49.59	C
ATOM	3342	NE1	TRP	C	144	54.499	95.932	56.913	1.00	49.59	C
ATOM	3343	CZ2	TRP	C	144	52.734	95.333	55.223	1.00	49.59	C
ATOM	3344	CZ3	TRP	C	144	52.604	96.937	53.409	1.00	49.59	C
ATOM	3345	CH2	TRP	C	144	52.169	95.759	54.047	1.00	49.59	C
ATOM	3346	C	TRP	C	144	57.356	100.055	53.730	1.00	57.36	C
ATOM	3347	O	TRP	C	144	56.619	101.025	53.561	1.00	57.36	C
ATOM	3348	N	TYR	C	145	58.644	100.055	53.406	1.00	52.11	C
ATOM	3349	CA	TYR	C	145	59.263	101.187	52.738	1.00	52.11	C
ATOM	3350	CB	TYR	C	145	60.785	101.147	52.863	1.00	49.32	C
ATOM	3351	CG	TYR	C	145	61.349	101.742	54.122	1.00	49.32	C
ATOM	3352	CD1	TYR	C	145	61.249	101.079	55.342	1.00	49.32	C
ATOM	3353	CE1	TYR	C	145	61.802	101.623	56.504	1.00	49.32	C
ATOM	3354	CD2	TYR	C	145	62.008	102.964	54.090	1.00	49.32	C
ATOM	3355	CE2	TYR	C	145	62.560	103.516	55.240	1.00	49.32	C
ATOM	3356	CZ	TYR	C	145	62.456	102.843	56.441	1.00	49.32	C
ATOM	3357	OH	TYR	C	145	63.017	103.394	57.570	1.00	49.32	C
ATOM	3358	C	TYR	C	145	58.908	100.977	51.269	1.00	52.11	C
ATOM	3359	O	TYR	C	145	58.761	99.840	50.819	1.00	52.11	C
ATOM	3360	N	ASN	C	146	58.755	102.061	50.524	1.00	46.62	C
ATOM	3361	CA	ASN	C	146	58.451	101.947	49.107	1.00	46.62	C
ATOM	3362	CB	ASN	C	146	57.070	102.513	48.779	1.00	47.96	C
ATOM	3363	CG	ASN	C	146	55.984	101.963	49.666	1.00	47.96	C
ATOM	3364	OD1	ASN	C	146	55.822	100.750	49.791	1.00	47.96	C
ATOM	3365	ND2	ASN	C	146	55.220	102.857	50.283	1.00	47.96	C
ATOM	3366	C	ASN	C	146	59.476	102.761	48.346	1.00	46.62	C
ATOM	3367	O	ASN	C	146	60.332	103.428	48.941	1.00	46.62	C
ATOM	3368	N	THR	C	147	59.401	102.673	47.025	1.00	45.12	C
ATOM	3369	CA	THR	C	147	60.259	103.461	46.164	1.00	45.12	C

FIGURE 2 Continued

ATOM	3370	CB	THR	C	147	61.132	102.623	45.199	1.00	38.21	C
ATOM	3371	OG1	THR	C	147	60.297	101.774	44.399	1.00	38.21	C
ATOM	3372	CG2	THR	C	147	62.151	101.808	45.969	1.00	38.21	C
ATOM	3373	C	THR	C	147	59.249	104.225	45.342	1.00	45.12	C
ATOM	3374	O	THR	C	147	58.133	103.750	45.111	1.00	45.12	C
ATOM	3375	N	TYR	C	148	59.639	105.416	44.922	1.00	38.47	C
ATOM	3376	CA	TYR	C	148	58.781	106.260	44.126	1.00	38.47	C
ATOM	3377	CB	TYR	C	148	58.378	107.477	44.954	1.00	38.18	C
ATOM	3378	CG	TYR	C	148	57.494	107.098	46.113	1.00	38.18	C
ATOM	3379	CD1	TYR	C	148	56.109	107.047	45.968	1.00	38.18	C
ATOM	3380	CE1	TYR	C	148	55.298	106.599	46.989	1.00	38.18	C
ATOM	3381	CD2	TYR	C	148	58.042	106.693	47.322	1.00	38.18	C
ATOM	3382	CE2	TYR	C	148	57.238	106.236	48.359	1.00	38.18	C
ATOM	3383	CZ	TYR	C	148	55.870	106.190	48.184	1.00	38.18	C
ATOM	3384	OH	TYR	C	148	55.072	105.723	49.197	1.00	38.18	C
ATOM	3385	C	TYR	C	148	59.610	106.648	42.933	1.00	38.47	C
ATOM	3386	O	TYR	C	148	60.638	107.303	43.068	1.00	38.47	C
ATOM	3387	N	SER	C	149	59.183	106.221	41.755	1.00	40.04	C
ATOM	3388	CA	SER	C	149	59.933	106.546	40.557	1.00	40.04	C
ATOM	3389	CB	SER	C	149	60.432	105.273	39.872	1.00	43.44	C
ATOM	3390	OG	SER	C	149	59.375	104.635	39.181	1.00	43.44	C
ATOM	3391	C	SER	C	149	59.035	107.303	39.615	1.00	40.04	C
ATOM	3392	O	SER	C	149	57.825	107.099	39.610	1.00	40.04	C
ATOM	3393	N	SER	C	150	59.630	108.191	38.828	1.00	43.81	C
ATOM	3394	CA	SER	C	150	58.873	108.959	37.860	1.00	43.81	C
ATOM	3395	CB	SER	C	150	59.799	109.869	37.060	1.00	37.57	C
ATOM	3396	OG	SER	C	150	59.130	110.395	35.918	1.00	37.57	C
ATOM	3397	C	SER	C	150	58.184	107.987	36.914	1.00	43.81	C
ATOM	3398	O	SER	C	150	58.746	106.957	36.531	1.00	43.81	C
ATOM	3399	N	ASN	C	151	56.962	108.319	36.539	1.00	40.85	C
ATOM	3400	CA	ASN	C	151	56.205	107.486	35.632	1.00	40.85	C
ATOM	3401	CB	ASN	C	151	54.745	107.446	36.073	1.00	48.31	C
ATOM	3402	CG	ASN	C	151	53.958	106.377	35.364	1.00	48.31	C
ATOM	3403	OD1	ASN	C	151	54.349	105.211	35.356	1.00	48.31	C
ATOM	3404	ND2	ASN	C	151	52.844	106.762	34.770	1.00	48.31	C
ATOM	3405	C	ASN	C	151	56.323	108.110	34.246	1.00	40.85	C
ATOM	3406	O	ASN	C	151	55.640	107.718	33.312	1.00	40.85	C
ATOM	3407	N	LEU	C	152	57.216	109.080	34.121	1.00	40.06	C
ATOM	3408	CA	LEU	C	152	57.405	109.780	32.861	1.00	40.06	C
ATOM	3409	CB	LEU	C	152	56.957	111.232	33.034	1.00	41.49	C
ATOM	3410	CG	LEU	C	152	57.124	112.179	31.855	1.00	41.49	C
ATOM	3411	CD1	LEU	C	152	56.460	111.593	30.617	1.00	41.49	C
ATOM	3412	CD2	LEU	C	152	56.506	113.520	32.218	1.00	41.49	C
ATOM	3413	C	LEU	C	152	58.840	109.752	32.345	1.00	40.06	C
ATOM	3414	O	LEU	C	152	59.073	109.688	31.146	1.00	40.06	C
ATOM	3415	N	TYR	C	153	59.802	109.800	33.252	1.00	43.87	C
ATOM	3416	CA	TYR	C	153	61.193	109.816	32.839	1.00	43.87	C
ATOM	3417	CB	TYR	C	153	61.866	111.075	33.372	1.00	35.17	C
ATOM	3418	CG	TYR	C	153	61.189	112.317	32.860	1.00	35.17	C
ATOM	3419	CD1	TYR	C	153	61.026	112.521	31.483	1.00	35.17	C
ATOM	3420	CE1	TYR	C	153	60.382	113.657	30.994	1.00	35.17	C
ATOM	3421	CD2	TYR	C	153	60.692	113.279	33.738	1.00	35.17	C
ATOM	3422	CE2	TYR	C	153	60.050	114.417	33.261	1.00	35.17	C
ATOM	3423	CZ	TYR	C	153	59.898	114.601	31.890	1.00	35.17	C
ATOM	3424	OH	TYR	C	153	59.269	115.724	31.413	1.00	35.17	C
ATOM	3425	C	TYR	C	153	61.949	108.589	33.272	1.00	43.87	C
ATOM	3426	O	TYR	C	153	61.646	107.994	34.304	1.00	43.87	C

FIGURE 2 Continued

ATOM	3427	N	LYS	C	154	62.939	108.218	32.471	1.00	45.23	C
ATOM	3428	CA	LYS	C	154	63.742	107.036	32.744	1.00	45.23	C
ATOM	3429	CB	LYS	C	154	62.946	105.784	32.376	1.00	55.04	C
ATOM	3430	CG	LYS	C	154	62.530	105.792	30.921	1.00	55.04	C
ATOM	3431	CD	LYS	C	154	62.062	104.444	30.432	1.00	55.04	C
ATOM	3432	CE	LYS	C	154	61.727	104.521	28.948	1.00	55.04	C
ATOM	3433	NZ	LYS	C	154	61.382	103.186	28.370	1.00	55.04	C
ATOM	3434	C	LYS	C	154	65.021	107.042	31.918	1.00	45.23	C
ATOM	3435	O	LYS	C	154	65.247	107.932	31.098	1.00	45.23	C
ATOM	3436	N	HIS	C	155	65.849	106.032	32.154	1.00	43.29	C
ATOM	3437	CA	HIS	C	155	67.082	105.840	31.407	1.00	43.29	C
ATOM	3438	CB	HIS	C	155	68.026	104.935	32.192	1.00	45.88	C
ATOM	3439	CG	HIS	C	155	68.584	105.569	33.428	1.00	45.88	C
ATOM	3440	CD2	HIS	C	155	68.266	105.409	34.735	1.00	45.88	C
ATOM	3441	ND1	HIS	C	155	69.597	106.503	33.392	1.00	45.88	C
ATOM	3442	CE1	HIS	C	155	69.881	106.891	34.624	1.00	45.88	C
ATOM	3443	NE2	HIS	C	155	69.086	106.243	35.458	1.00	45.88	C
ATOM	3444	C	HIS	C	155	66.621	105.133	30.135	1.00	43.29	C
ATOM	3445	O	HIS	C	155	66.205	103.980	30.187	1.00	43.29	C
ATOM	3446	N	VAL	C	156	66.665	105.825	29.001	1.00	41.62	C
ATOM	3447	CA	VAL	C	156	66.216	105.241	27.743	1.00	41.62	C
ATOM	3448	CB	VAL	C	156	66.141	106.293	26.619	1.00	38.44	C
ATOM	3449	CG1	VAL	C	156	65.068	107.330	26.938	1.00	38.44	C
ATOM	3450	CG2	VAL	C	156	67.508	106.952	26.435	1.00	38.44	C
ATOM	3451	C	VAL	C	156	67.082	104.097	27.234	1.00	41.62	C
ATOM	3452	O	VAL	C	156	66.609	103.257	26.475	1.00	41.62	C
ATOM	3453	N	ASP	C	157	68.343	104.053	27.643	1.00	42.66	C
ATOM	3454	CA	ASP	C	157	69.233	103.000	27.170	1.00	42.66	C
ATOM	3455	CB	ASP	C	157	70.695	103.466	27.267	1.00	47.85	C
ATOM	3456	CG	ASP	C	157	71.116	103.810	28.691	1.00	47.85	C
ATOM	3457	OD1	ASP	C	157	70.240	104.155	29.513	1.00	47.85	C
ATOM	3458	OD2	ASP	C	157	72.332	103.751	28.984	1.00	47.85	C
ATOM	3459	C	ASP	C	157	69.050	101.667	27.888	1.00	42.66	C
ATOM	3460	O	ASP	C	157	69.129	100.608	27.263	1.00	42.66	C
ATOM	3461	N	THR	C	158	68.795	101.720	29.191	1.00	45.51	C
ATOM	3462	CA	THR	C	158	68.617	100.511	29.985	1.00	45.51	C
ATOM	3463	CB	THR	C	158	69.473	100.560	31.267	1.00	52.41	C
ATOM	3464	OG1	THR	C	158	68.983	101.595	32.130	1.00	52.41	C
ATOM	3465	CG2	THR	C	158	70.932	100.838	30.925	1.00	52.41	C
ATOM	3466	C	THR	C	158	67.165	100.301	30.394	1.00	45.51	C
ATOM	3467	O	THR	C	158	66.781	99.214	30.819	1.00	45.51	C
ATOM	3468	N	GLY	C	159	66.359	101.345	30.268	1.00	41.78	C
ATOM	3469	CA	GLY	C	159	64.965	101.238	30.643	1.00	41.78	C
ATOM	3470	C	GLY	C	159	64.757	101.414	32.136	1.00	41.78	C
ATOM	3471	O	GLY	C	159	63.618	101.533	32.593	1.00	41.78	C
ATOM	3472	N	ARG	C	160	65.845	101.436	32.903	1.00	39.85	C
ATOM	3473	CA	ARG	C	160	65.734	101.606	34.347	1.00	39.85	C
ATOM	3474	CB	ARG	C	160	67.095	101.393	35.010	1.00	69.78	C
ATOM	3475	CG	ARG	C	160	67.652	100.006	34.724	1.00	69.78	C
ATOM	3476	CD	ARG	C	160	68.850	99.647	35.586	1.00	69.78	C
ATOM	3477	NE	ARG	C	160	68.460	99.291	36.944	1.00	69.78	C
ATOM	3478	CZ	ARG	C	160	69.316	98.944	37.898	1.00	69.78	C
ATOM	3479	NH1	ARG	C	160	70.621	98.903	37.643	1.00	69.78	C
ATOM	3480	NH2	ARG	C	160	68.870	98.642	39.110	1.00	69.78	C
ATOM	3481	C	ARG	C	160	65.128	102.967	34.718	1.00	39.85	C
ATOM	3482	O	ARG	C	160	65.246	103.952	33.978	1.00	39.85	C
ATOM	3483	N	ARG	C	161	64.479	102.994	35.877	1.00	39.91	C

FIGURE 2 Continued

ATOM	3484	CA	ARG	C	161	63.760	104.161	36.397	1.00	39.91	C
ATOM	3485	CB	ARG	C	161	62.639	103.640	37.295	1.00	51.78	C
ATOM	3486	CG	ARG	C	161	61.673	102.773	36.529	1.00	51.78	C
ATOM	3487	CD	ARG	C	161	60.928	103.678	35.593	1.00	51.78	C
ATOM	3488	NE	ARG	C	161	60.408	103.015	34.418	1.00	51.78	C
ATOM	3489	CZ	ARG	C	161	59.597	103.608	33.548	1.00	51.78	C
ATOM	3490	NH1	ARG	C	161	59.224	104.873	33.742	1.00	51.78	C
ATOM	3491	NH2	ARG	C	161	59.166	102.939	32.482	1.00	51.78	C
ATOM	3492	C	ARG	C	161	64.509	105.269	37.135	1.00	39.91	C
ATOM	3493	O	ARG	C	161	65.636	105.089	37.573	1.00	39.91	C
ATOM	3494	N	TYR	C	162	63.854	106.423	37.248	1.00	39.62	C
ATOM	3495	CA	TYR	C	162	64.378	107.583	37.978	1.00	39.62	C
ATOM	3496	CB	TYR	C	162	64.043	108.894	37.272	1.00	43.92	C
ATOM	3497	CG	TYR	C	162	64.828	109.224	36.027	1.00	43.92	C
ATOM	3498	CD1	TYR	C	162	65.860	108.407	35.568	1.00	43.92	C
ATOM	3499	CE1	TYR	C	162	66.576	108.742	34.417	1.00	43.92	C
ATOM	3500	CD2	TYR	C	162	64.536	110.378	35.302	1.00	43.92	C
ATOM	3501	CE2	TYR	C	162	65.239	110.714	34.164	1.00	43.92	C
ATOM	3502	CZ	TYR	C	162	66.253	109.900	33.725	1.00	43.92	C
ATOM	3503	OH	TYR	C	162	66.938	110.259	32.591	1.00	43.92	C
ATOM	3504	C	TYR	C	162	63.647	107.580	39.322	1.00	39.62	C
ATOM	3505	O	TYR	C	162	62.426	107.748	39.361	1.00	39.62	C
ATOM	3506	N	TYR	C	163	64.386	107.406	40.413	1.00	37.53	C
ATOM	3507	CA	TYR	C	163	63.796	107.353	41.747	1.00	37.53	C
ATOM	3508	CB	TYR	C	163	64.380	106.174	42.536	1.00	45.85	C
ATOM	3509	CG	TYR	C	163	63.990	104.836	41.964	1.00	45.85	C
ATOM	3510	CD1	TYR	C	163	64.654	104.303	40.860	1.00	45.85	C
ATOM	3511	CE1	TYR	C	163	64.219	103.123	40.264	1.00	45.85	C
ATOM	3512	CD2	TYR	C	163	62.888	104.145	42.466	1.00	45.85	C
ATOM	3513	CE2	TYR	C	163	62.446	102.968	41.881	1.00	45.85	C
ATOM	3514	CZ	TYR	C	163	63.108	102.464	40.780	1.00	45.85	C
ATOM	3515	OH	TYR	C	163	62.624	101.328	40.172	1.00	45.85	C
ATOM	3516	C	TYR	C	163	63.929	108.610	42.593	1.00	37.53	C
ATOM	3517	O	TYR	C	163	64.946	109.309	42.547	1.00	37.53	C
ATOM	3518	N	VAL	C	164	62.873	108.880	43.364	1.00	34.97	C
ATOM	3519	CA	VAL	C	164	62.828	110.001	44.290	1.00	34.97	C
ATOM	3520	CB	VAL	C	164	61.439	110.111	44.968	1.00	31.66	C
ATOM	3521	CG1	VAL	C	164	61.479	111.154	46.086	1.00	31.66	C
ATOM	3522	CG2	VAL	C	164	60.378	110.483	43.938	1.00	31.66	C
ATOM	3523	C	VAL	C	164	63.849	109.598	45.341	1.00	34.97	C
ATOM	3524	O	VAL	C	164	63.898	108.439	45.733	1.00	34.97	C
ATOM	3525	N	ALA	C	165	64.669	110.531	45.806	1.00	36.75	C
ATOM	3526	CA	ALA	C	165	65.672	110.165	46.794	1.00	36.75	C
ATOM	3527	CB	ALA	C	165	66.783	109.359	46.113	1.00	31.20	C
ATOM	3528	C	ALA	C	165	66.276	111.340	47.541	1.00	36.75	C
ATOM	3529	O	ALA	C	165	66.374	112.439	47.013	1.00	36.75	C
ATOM	3530	N	LEU	C	166	66.674	111.086	48.781	1.00	44.55	C
ATOM	3531	CA	LEU	C	166	67.311	112.090	49.626	1.00	44.55	C
ATOM	3532	CB	LEU	C	166	66.497	112.337	50.905	1.00	33.70	C
ATOM	3533	CG	LEU	C	166	65.128	112.988	50.687	1.00	33.70	C
ATOM	3534	CD1	LEU	C	166	64.403	113.171	52.016	1.00	33.70	C
ATOM	3535	CD2	LEU	C	166	65.316	114.328	49.995	1.00	33.70	C
ATOM	3536	C	LEU	C	166	68.672	111.521	49.985	1.00	44.55	C
ATOM	3537	O	LEU	C	166	68.784	110.349	50.348	1.00	44.55	C
ATOM	3538	N	ASN	C	167	69.708	112.341	49.882	1.00	46.44	C
ATOM	3539	CA	ASN	C	167	71.053	111.877	50.202	1.00	46.44	C
ATOM	3540	CB	ASN	C	167	72.083	112.851	49.631	1.00	43.06	C

FIGURE 2 Continued

ATOM	3541	CG	ASN	C	167	72.140	112.799	48.124	1.00	43.06	C
ATOM	3542	OD1	ASN	C	167	72.416	111.748	47.549	1.00	43.06	C
ATOM	3543	ND2	ASN	C	167	71.873	113.925	47.473	1.00	43.06	C
ATOM	3544	C	ASN	C	167	71.307	111.664	51.696	1.00	46.44	C
ATOM	3545	O	ASN	C	167	70.527	112.106	52.545	1.00	46.44	C
ATOM	3546	N	LYS	C	168	72.407	110.976	52.001	1.00	66.98	C
ATOM	3547	CA	LYS	C	168	72.798	110.689	53.380	1.00	66.98	C
ATOM	3548	CB	LYS	C	168	74.184	110.041	53.412	1.00	99.56	C
ATOM	3549	CG	LYS	C	168	74.278	108.744	52.628	1.00	99.56	C
ATOM	3550	CD	LYS	C	168	75.692	108.186	52.634	1.00	99.56	C
ATOM	3551	CE	LYS	C	168	75.790	106.924	51.788	1.00	99.56	C
ATOM	3552	NZ	LYS	C	168	77.184	106.400	51.741	1.00	99.56	C
ATOM	3553	C	LYS	C	168	72.820	111.963	54.212	1.00	66.98	C
ATOM	3554	O	LYS	C	168	72.720	111.913	55.436	1.00	66.98	C
ATOM	3555	N	ASP	C	169	72.944	113.104	53.539	1.00	53.34	C
ATOM	3556	CA	ASP	C	169	72.982	114.393	54.214	1.00	53.34	C
ATOM	3557	CB	ASP	C	169	74.044	115.289	53.565	1.00	62.36	C
ATOM	3558	CG	ASP	C	169	73.620	115.806	52.203	1.00	62.36	C
ATOM	3559	OD1	ASP	C	169	72.801	115.134	51.541	1.00	62.36	C
ATOM	3560	OD2	ASP	C	169	74.112	116.879	51.787	1.00	62.36	C
ATOM	3561	C	ASP	C	169	71.622	115.097	54.199	1.00	53.34	C
ATOM	3562	O	ASP	C	169	71.495	116.221	54.684	1.00	53.34	C
ATOM	3563	N	GLY	C	170	70.609	114.447	53.635	1.00	56.33	C
ATOM	3564	CA	GLY	C	170	69.288	115.050	53.599	1.00	56.33	C
ATOM	3565	C	GLY	C	170	68.960	115.919	52.395	1.00	56.33	C
ATOM	3566	O	GLY	C	170	67.831	116.379	52.258	1.00	56.33	C
ATOM	3567	N	THR	C	171	69.930	116.159	51.523	1.00	45.41	C
ATOM	3568	CA	THR	C	171	69.685	116.967	50.334	1.00	45.41	C
ATOM	3569	CB	THR	C	171	70.984	117.567	49.769	1.00	41.09	C
ATOM	3570	OG1	THR	C	171	71.881	116.505	49.411	1.00	41.09	C
ATOM	3571	CG2	THR	C	171	71.639	118.476	50.792	1.00	41.09	C
ATOM	3572	C	THR	C	171	69.071	116.107	49.238	1.00	45.41	C
ATOM	3573	O	THR	C	171	69.305	114.895	49.179	1.00	45.41	C
ATOM	3574	N	PRO	C	172	68.260	116.719	48.364	1.00	46.08	C
ATOM	3575	CD	PRO	C	172	67.762	118.105	48.390	1.00	39.25	C
ATOM	3576	CA	PRO	C	172	67.636	115.965	47.277	1.00	46.08	C
ATOM	3577	CB	PRO	C	172	66.656	116.968	46.679	1.00	39.25	C
ATOM	3578	CG	PRO	C	172	67.302	118.290	46.970	1.00	39.25	C
ATOM	3579	C	PRO	C	172	68.665	115.485	46.261	1.00	46.08	C
ATOM	3580	O	PRO	C	172	69.519	116.255	45.820	1.00	46.08	C
ATOM	3581	N	ARG	C	173	68.574	114.206	45.903	1.00	42.90	C
ATOM	3582	CA	ARG	C	173	69.479	113.598	44.938	1.00	42.90	C
ATOM	3583	CB	ARG	C	173	69.773	112.149	45.334	1.00	59.68	C
ATOM	3584	CG	ARG	C	173	70.917	111.513	44.565	1.00	59.68	C
ATOM	3585	CD	ARG	C	173	71.158	110.080	45.016	1.00	59.68	C
ATOM	3586	NE	ARG	C	173	72.291	109.465	44.329	1.00	59.68	C
ATOM	3587	CZ	ARG	C	173	73.567	109.787	44.538	1.00	59.68	C
ATOM	3588	NH1	ARG	C	173	73.889	110.721	45.424	1.00	59.68	C
ATOM	3589	NH2	ARG	C	173	74.525	109.185	43.847	1.00	59.68	C
ATOM	3590	C	ARG	C	173	68.819	113.631	43.567	1.00	42.90	C
ATOM	3591	O	ARG	C	173	67.596	113.679	43.464	1.00	42.90	C
ATOM	3592	N	GLU	C	174	69.625	113.618	42.513	1.00	45.54	C
ATOM	3593	CA	GLU	C	174	69.081	113.628	41.164	1.00	45.54	C
ATOM	3594	CB	GLU	C	174	70.181	113.942	40.155	1.00	99.99	C
ATOM	3595	CG	GLU	C	174	70.694	115.359	40.240	1.00	99.99	C
ATOM	3596	CD	GLU	C	174	71.941	115.565	39.418	1.00	99.99	C
ATOM	3597	OE1	GLU	C	174	72.997	115.018	39.802	1.00	99.99	C

FIGURE 2 Continued

ATOM	3598	OE2	GLU	C	174	71.864	116.268	38.387	1.00	99.99	C
ATOM	3599	C	GLU	C	174	68.483	112.260	40.865	1.00	45.54	C
ATOM	3600	O	GLU	C	174	69.078	111.228	41.190	1.00	45.54	C
ATOM	3601	N	GLY	C	175	67.303	112.255	40.254	1.00	48.09	C
ATOM	3602	CA	GLY	C	175	66.652	111.002	39.923	1.00	48.09	C
ATOM	3603	C	GLY	C	175	67.429	110.165	38.923	1.00	48.09	C
ATOM	3604	O	GLY	C	175	67.243	108.950	38.850	1.00	48.09	C
ATOM	3605	N	THR	C	176	68.297	110.814	38.150	1.00	45.73	C
ATOM	3606	CA	THR	C	176	69.100	110.126	37.145	1.00	45.73	C
ATOM	3607	CB	THR	C	176	69.703	111.109	36.129	1.00	35.76	C
ATOM	3608	OG1	THR	C	176	70.482	112.087	36.827	1.00	35.76	C
ATOM	3609	CG2	THR	C	176	68.612	111.794	35.320	1.00	35.76	C
ATOM	3610	C	THR	C	176	70.254	109.350	37.772	1.00	45.73	C
ATOM	3611	O	THR	C	176	70.929	108.576	37.092	1.00	45.73	C
ATOM	3612	N	ARG	C	177	70.470	109.553	39.066	1.00	50.01	C
ATOM	3613	CA	ARG	C	177	71.549	108.880	39.776	1.00	50.01	C
ATOM	3614	CB	ARG	C	177	72.503	109.918	40.370	1.00	67.80	C
ATOM	3615	CG	ARG	C	177	73.068	110.895	39.349	1.00	67.80	C
ATOM	3616	CD	ARG	C	177	74.077	111.823	40.001	1.00	67.80	C
ATOM	3617	NE	ARG	C	177	75.105	111.060	40.700	1.00	67.80	C
ATOM	3618	CZ	ARG	C	177	75.975	111.580	41.559	1.00	67.80	C
ATOM	3619	NH1	ARG	C	177	75.947	112.879	41.828	1.00	67.80	C
ATOM	3620	NH2	ARG	C	177	76.862	110.795	42.161	1.00	67.80	C
ATOM	3621	C	ARG	C	177	70.995	107.995	40.886	1.00	50.01	C
ATOM	3622	O	ARG	C	177	71.487	108.016	42.016	1.00	50.01	C
ATOM	3623	N	THR	C	178	69.978	107.205	40.563	1.00	45.45	C
ATOM	3624	CA	THR	C	178	69.355	106.345	41.564	1.00	45.45	C
ATOM	3625	CB	THR	C	178	68.033	106.948	42.043	1.00	33.70	C
ATOM	3626	OG1	THR	C	178	67.175	107.134	40.908	1.00	33.70	C
ATOM	3627	CG2	THR	C	178	68.270	108.290	42.723	1.00	33.70	C
ATOM	3628	C	THR	C	178	69.046	104.949	41.057	1.00	45.45	C
ATOM	3629	O	THR	C	178	68.777	104.746	39.871	1.00	45.45	C
ATOM	3630	N	LYS	C	179	69.085	103.985	41.966	1.00	42.46	C
ATOM	3631	CA	LYS	C	179	68.768	102.607	41.629	1.00	42.46	C
ATOM	3632	CB	LYS	C	179	70.042	101.765	41.558	1.00	71.18	C
ATOM	3633	CG	LYS	C	179	70.915	102.133	40.373	1.00	71.18	C
ATOM	3634	CD	LYS	C	179	72.081	101.174	40.190	1.00	71.18	C
ATOM	3635	CE	LYS	C	179	72.936	101.569	38.981	1.00	71.18	C
ATOM	3636	NZ	LYS	C	179	74.059	100.617	38.729	1.00	71.18	C
ATOM	3637	C	LYS	C	179	67.798	102.072	42.684	1.00	42.46	C
ATOM	3638	O	LYS	C	179	68.010	102.235	43.893	1.00	42.46	C
ATOM	3639	N	ARG	C	180	66.724	101.450	42.211	1.00	51.30	C
ATOM	3640	CA	ARG	C	180	65.692	100.906	43.078	1.00	51.30	C
ATOM	3641	CB	ARG	C	180	64.901	99.817	42.345	1.00	47.59	C
ATOM	3642	CG	ARG	C	180	63.857	99.129	43.223	1.00	47.59	C
ATOM	3643	CD	ARG	C	180	63.351	97.875	42.573	1.00	47.59	C
ATOM	3644	NE	ARG	C	180	62.601	98.150	41.352	1.00	47.59	C
ATOM	3645	CZ	ARG	C	180	61.343	98.583	41.327	1.00	47.59	C
ATOM	3646	NH1	ARG	C	180	60.691	98.793	42.466	1.00	47.59	C
ATOM	3647	NH2	ARG	C	180	60.735	98.795	40.163	1.00	47.59	C
ATOM	3648	C	ARG	C	180	66.149	100.341	44.418	1.00	51.30	C
ATOM	3649	O	ARG	C	180	65.505	100.573	45.434	1.00	51.30	C
ATOM	3650	N	HIS	C	181	67.253	99.608	44.435	1.00	50.09	C
ATOM	3651	CA	HIS	C	181	67.705	98.996	45.680	1.00	50.09	C
ATOM	3652	CB	HIS	C	181	68.424	97.685	45.373	1.00	70.93	C
ATOM	3653	CG	HIS	C	181	67.570	96.701	44.637	1.00	70.93	C
ATOM	3654	CD2	HIS	C	181	67.751	96.069	43.454	1.00	70.93	C

FIGURE 2 Continued

ATOM	3655	ND1	HIS	C	181	66.339	96.294	45.105	1.00	70.93	C
ATOM	3656	CE1	HIS	C	181	65.798	95.454	44.241	1.00	70.93	C
ATOM	3657	NE2	HIS	C	181	66.635	95.301	43.230	1.00	70.93	C
ATOM	3658	C	HIS	C	181	68.554	99.842	46.607	1.00	50.09	C
ATOM	3659	O	HIS	C	181	68.812	99.440	47.738	1.00	50.09	C
ATOM	3660	N	GLN	C	182	68.986	101.012	46.150	1.00	53.85	C
ATOM	3661	CA	GLN	C	182	69.802	101.881	46.996	1.00	53.85	C
ATOM	3662	CB	GLN	C	182	70.357	103.049	46.176	1.00	61.78	C
ATOM	3663	CG	GLN	C	182	71.310	102.612	45.078	1.00	61.78	C
ATOM	3664	CD	GLN	C	182	71.881	103.773	44.284	1.00	61.78	C
ATOM	3665	OE1	GLN	C	182	71.174	104.429	43.514	1.00	61.78	C
ATOM	3666	NE2	GLN	C	182	73.170	104.035	44.472	1.00	61.78	C
ATOM	3667	C	GLN	C	182	68.985	102.399	48.182	1.00	53.85	C
ATOM	3668	O	GLN	C	182	67.777	102.623	48.078	1.00	53.85	C
ATOM	3669	N	LYS	C	183	69.663	102.582	49.308	1.00	54.51	C
ATOM	3670	CA	LYS	C	183	69.047	103.051	50.548	1.00	54.51	C
ATOM	3671	CB	LYS	C	183	70.130	103.130	51.629	1.00	77.75	C
ATOM	3672	CG	LYS	C	183	69.647	103.424	53.033	1.00	77.75	C
ATOM	3673	CD	LYS	C	183	70.825	103.403	54.011	1.00	77.75	C
ATOM	3674	CE	LYS	C	183	70.393	103.704	55.443	1.00	77.75	C
ATOM	3675	NZ	LYS	C	183	71.526	103.617	56.411	1.00	77.75	C
ATOM	3676	C	LYS	C	183	68.307	104.392	50.442	1.00	54.51	C
ATOM	3677	O	LYS	C	183	67.215	104.542	50.988	1.00	54.51	C
ATOM	3678	N	PHE	C	184	68.878	105.357	49.725	1.00	47.10	C
ATOM	3679	CA	PHE	C	184	68.243	106.670	49.614	1.00	47.10	C
ATOM	3680	CB	PHE	C	184	69.262	107.727	49.168	1.00	60.40	C
ATOM	3681	CG	PHE	C	184	70.100	107.325	47.995	1.00	60.40	C
ATOM	3682	CD1	PHE	C	184	69.526	106.748	46.867	1.00	60.40	C
ATOM	3683	CD2	PHE	C	184	71.468	107.583	47.995	1.00	60.40	C
ATOM	3684	CE1	PHE	C	184	70.302	106.433	45.747	1.00	60.40	C
ATOM	3685	CE2	PHE	C	184	72.256	107.276	46.882	1.00	60.40	C
ATOM	3686	CZ	PHE	C	184	71.670	106.699	45.754	1.00	60.40	C
ATOM	3687	C	PHE	C	184	66.984	106.786	48.757	1.00	47.10	C
ATOM	3688	O	PHE	C	184	66.435	107.874	48.612	1.00	47.10	C
ATOM	3689	N	THR	C	185	66.528	105.670	48.196	1.00	41.07	C
ATOM	3690	CA	THR	C	185	65.325	105.655	47.367	1.00	41.07	C
ATOM	3691	CB	THR	C	185	65.539	104.852	46.066	1.00	41.06	C
ATOM	3692	OG1	THR	C	185	65.820	103.485	46.390	1.00	41.06	C
ATOM	3693	CG2	THR	C	185	66.692	105.431	45.254	1.00	41.06	C
ATOM	3694	C	THR	C	185	64.188	104.991	48.145	1.00	41.07	C
ATOM	3695	O	THR	C	185	63.075	104.837	47.639	1.00	41.07	C
ATOM	3696	N	HIS	C	186	64.476	104.595	49.381	1.00	41.75	C
ATOM	3697	CA	HIS	C	186	63.479	103.931	50.211	1.00	41.75	C
ATOM	3698	CB	HIS	C	186	64.139	102.810	51.018	1.00	62.27	C
ATOM	3699	CG	HIS	C	186	64.809	101.772	50.170	1.00	62.27	C
ATOM	3700	CD2	HIS	C	186	64.964	101.681	48.827	1.00	62.27	C
ATOM	3701	ND1	HIS	C	186	65.429	100.661	50.701	1.00	62.27	C
ATOM	3702	CE1	HIS	C	186	65.936	99.932	49.723	1.00	62.27	C
ATOM	3703	NE2	HIS	C	186	65.668	100.529	48.577	1.00	62.27	C
ATOM	3704	C	HIS	C	186	62.770	104.905	51.145	1.00	41.75	C
ATOM	3705	O	HIS	C	186	63.398	105.558	51.975	1.00	41.75	C
ATOM	3706	N	PHE	C	187	61.452	104.991	51.007	1.00	38.60	C
ATOM	3707	CA	PHE	C	187	60.670	105.898	51.831	1.00	38.60	C
ATOM	3708	CB	PHE	C	187	60.068	107.017	50.969	1.00	39.11	C
ATOM	3709	CG	PHE	C	187	61.084	108.010	50.464	1.00	39.11	C
ATOM	3710	CD1	PHE	C	187	61.869	107.723	49.348	1.00	39.11	C
ATOM	3711	CD2	PHE	C	187	61.269	109.224	51.117	1.00	39.11	C

FIGURE 2 Continued

ATOM	3712	CE1	PHE	C	187	62.824	108.630	48.887	1.00	39.11	C
ATOM	3713	CE2	PHE	C	187	62.226	110.142	50.661	1.00	39.11	C
ATOM	3714	CZ	PHE	C	187	63.004	109.839	49.542	1.00	39.11	C
ATOM	3715	C	PHE	C	187	59.565	105.182	52.587	1.00	38.60	C
ATOM	3716	O	PHE	C	187	58.882	104.318	52.044	1.00	38.60	C
ATOM	3717	N	LEU	C	188	59.390	105.555	53.848	1.00	47.29	C
ATOM	3718	CA	LEU	C	188	58.368	104.948	54.684	1.00	47.29	C
ATOM	3719	CB	LEU	C	188	58.979	104.517	56.020	1.00	52.27	C
ATOM	3720	CG	LEU	C	188	58.046	103.951	57.094	1.00	52.27	C
ATOM	3721	CD1	LEU	C	188	57.445	102.640	56.629	1.00	52.27	C
ATOM	3722	CD2	LEU	C	188	58.831	103.741	58.378	1.00	52.27	C
ATOM	3723	C	LEU	C	188	57.216	105.915	54.936	1.00	47.29	C
ATOM	3724	O	LEU	C	188	57.392	106.966	55.557	1.00	47.29	C
ATOM	3725	N	PRO	C	189	56.023	105.591	54.422	1.00	47.58	C
ATOM	3726	CD	PRO	C	189	55.626	104.545	53.464	1.00	37.11	C
ATOM	3727	CA	PRO	C	189	54.922	106.515	54.676	1.00	47.58	C
ATOM	3728	CB	PRO	C	189	53.779	105.936	53.838	1.00	37.11	C
ATOM	3729	CG	PRO	C	189	54.486	105.213	52.731	1.00	37.11	C
ATOM	3730	C	PRO	C	189	54.644	106.436	56.173	1.00	47.58	C
ATOM	3731	O	PRO	C	189	54.253	105.391	56.683	1.00	47.58	C
ATOM	3732	N	ARG	C	190	54.888	107.528	56.878	1.00	53.62	C
ATOM	3733	CA	ARG	C	190	54.655	107.565	58.308	1.00	53.62	C
ATOM	3734	CB	ARG	C	190	55.822	108.261	59.017	1.00	57.94	C
ATOM	3735	CG	ARG	C	190	56.972	107.325	59.374	1.00	57.94	C
ATOM	3736	CD	ARG	C	190	58.217	108.077	59.830	1.00	57.94	C
ATOM	3737	NE	ARG	C	190	57.946	109.118	60.827	1.00	57.94	C
ATOM	3738	CZ	ARG	C	190	57.447	108.892	62.038	1.00	57.94	C
ATOM	3739	NH1	ARG	C	190	57.159	107.652	62.416	1.00	57.94	C
ATOM	3740	NH2	ARG	C	190	57.243	109.900	62.871	1.00	57.94	C
ATOM	3741	C	ARG	C	190	53.355	108.300	58.578	1.00	53.62	C
ATOM	3742	O	ARG	C	190	52.907	109.107	57.762	1.00	53.62	C
ATOM	3743	N	PRO	C	191	52.714	108.010	59.722	1.00	60.11	C
ATOM	3744	CD	PRO	C	191	53.045	106.930	60.669	1.00	55.97	C
ATOM	3745	CA	PRO	C	191	51.453	108.655	60.097	1.00	60.11	C
ATOM	3746	CB	PRO	C	191	50.887	107.701	61.138	1.00	55.97	C
ATOM	3747	CG	PRO	C	191	52.113	107.224	61.827	1.00	55.97	C
ATOM	3748	C	PRO	C	191	51.656	110.064	60.651	1.00	60.11	C
ATOM	3749	O	PRO	C	191	52.767	110.463	61.008	1.00	60.11	C
ATOM	3750	N	VAL	C	192	50.570	110.818	60.719	1.00	54.92	C
ATOM	3751	CA	VAL	C	192	50.637	112.177	61.231	1.00	54.92	C
ATOM	3752	CB	VAL	C	192	50.114	113.183	60.188	1.00	49.31	C
ATOM	3753	CG1	VAL	C	192	50.034	114.575	60.798	1.00	49.31	C
ATOM	3754	CG2	VAL	C	192	51.034	113.187	58.968	1.00	49.31	C
ATOM	3755	C	VAL	C	192	49.836	112.340	62.518	1.00	54.92	C
ATOM	3756	O	VAL	C	192	48.669	111.954	62.597	1.00	54.92	C
ATOM	3757	N	ASP	C	193	50.483	112.910	63.526	1.00	56.92	C
ATOM	3758	CA	ASP	C	193	49.851	113.159	64.814	1.00	56.92	C
ATOM	3759	CB	ASP	C	193	50.924	113.391	65.879	1.00	65.93	C
ATOM	3760	CG	ASP	C	193	50.371	113.347	67.289	1.00	65.93	C
ATOM	3761	OD1	ASP	C	193	49.235	113.825	67.512	1.00	65.93	C
ATOM	3762	OD2	ASP	C	193	51.089	112.840	68.179	1.00	65.93	C
ATOM	3763	C	ASP	C	193	49.004	114.424	64.661	1.00	56.92	C
ATOM	3764	O	ASP	C	193	49.523	115.485	64.298	1.00	56.92	C
ATOM	3765	N	PRO	C	194	47.694	114.329	64.937	1.00	79.75	C
ATOM	3766	CD	PRO	C	194	46.978	113.108	65.345	1.00	100.00	C
ATOM	3767	CA	PRO	C	194	46.765	115.460	64.831	1.00	79.75	C
ATOM	3768	CB	PRO	C	194	45.446	114.868	65.323	1.00	100.00	C

FIGURE 2 Continued

ATOM	3769	CG	PRO	C	194	45.560	113.429	64.953	1.00	100.00	C
ATOM	3770	C	PRO	C	194	47.184	116.672	65.664	1.00	79.75	C
ATOM	3771	O	PRO	C	194	47.107	117.817	65.210	1.00	79.75	C
ATOM	3772	N	ASP	C	195	47.635	116.405	66.884	1.00	70.88	C
ATOM	3773	CA	ASP	C	195	48.043	117.453	67.808	1.00	70.88	C
ATOM	3774	CB	ASP	C	195	48.136	116.877	69.220	1.00	92.45	C
ATOM	3775	CG	ASP	C	195	46.861	116.173	69.644	1.00	92.45	C
ATOM	3776	OD1	ASP	C	195	45.794	116.826	69.634	1.00	92.45	C
ATOM	3777	OD2	ASP	C	195	46.927	114.970	69.983	1.00	92.45	C
ATOM	3778	C	ASP	C	195	49.357	118.131	67.445	1.00	70.88	C
ATOM	3779	O	ASP	C	195	49.591	119.280	67.825	1.00	70.88	C
ATOM	3780	N	LYS	C	196	50.218	117.428	66.717	1.00	79.05	C
ATOM	3781	CA	LYS	C	196	51.504	117.996	66.328	1.00	79.05	C
ATOM	3782	CB	LYS	C	196	52.490	116.884	65.964	1.00	74.82	C
ATOM	3783	CG	LYS	C	196	52.750	115.883	67.072	1.00	74.82	C
ATOM	3784	CD	LYS	C	196	53.272	116.553	68.322	1.00	74.82	C
ATOM	3785	CE	LYS	C	196	53.425	115.545	69.454	1.00	74.82	C
ATOM	3786	NZ	LYS	C	196	53.707	116.210	70.766	1.00	74.82	C

FIGURE 2 Continued

ATOM	3787	C	LYS	C	196	51.356	118.957	65.150	1.00	79.05	C
ATOM	3788	O	LYS	C	196	52.226	119.801	64.918	1.00	79.05	C
ATOM	3789	N	VAL	C	197	50.250	118.829	64.417	1.00	61.75	C
ATOM	3790	CA	VAL	C	197	49.973	119.677	63.256	1.00	61.75	C
ATOM	3791	CB	VAL	C	197	49.442	118.832	62.083	1.00	88.39	C
ATOM	3792	CG1	VAL	C	197	49.254	119.704	60.855	1.00	88.39	C
ATOM	3793	CG2	VAL	C	197	50.391	117.695	61.797	1.00	88.39	C
ATOM	3794	C	VAL	C	197	48.924	120.748	63.585	1.00	61.75	C
ATOM	3795	O	VAL	C	197	47.724	120.493	63.493	1.00	61.75	C
ATOM	3796	N	PRO	C	198	49.362	121.960	63.967	1.00	68.67	C
ATOM	3797	CD	PRO	C	198	50.758	122.357	64.217	1.00	60.06	C
ATOM	3798	CA	PRO	C	198	48.449	123.058	64.310	1.00	68.67	C
ATOM	3799	CB	PRO	C	198	49.399	124.212	64.603	1.00	60.06	C
ATOM	3800	CG	PRO	C	198	50.591	123.513	65.172	1.00	60.06	C
ATOM	3801	C	PRO	C	198	47.436	123.410	63.225	1.00	68.67	C
ATOM	3802	O	PRO	C	198	46.257	123.607	63.506	1.00	68.67	C
ATOM	3803	N	GLU	C	199	47.899	123.484	61.985	1.00	73.27	C
ATOM	3804	CA	GLU	C	199	47.040	123.826	60.857	1.00	73.27	C
ATOM	3805	CB	GLU	C	199	47.890	123.905	59.593	1.00	100.00	C
ATOM	3806	CG	GLU	C	199	49.179	124.679	59.789	1.00	100.00	C
ATOM	3807	CD	GLU	C	199	48.940	126.062	60.360	1.00	100.00	C
ATOM	3808	OE1	GLU	C	199	48.209	126.851	59.721	1.00	100.00	C
ATOM	3809	OE2	GLU	C	199	49.483	126.358	61.447	1.00	100.00	C
ATOM	3810	C	GLU	C	199	45.874	122.859	60.624	1.00	73.27	C
ATOM	3811	O	GLU	C	199	44.870	123.221	60.014	1.00	73.27	C
ATOM	3812	N	LEU	C	200	46.003	121.633	61.114	1.00	90.93	C
ATOM	3813	CA	LEU	C	200	44.967	120.623	60.918	1.00	90.93	C
ATOM	3814	CB	LEU	C	200	45.221	119.409	61.817	1.00	63.86	C
ATOM	3815	CG	LEU	C	200	44.269	118.230	61.589	1.00	63.86	C
ATOM	3816	CD1	LEU	C	200	44.364	117.755	60.142	1.00	63.86	C
ATOM	3817	CD2	LEU	C	200	44.621	117.101	62.550	1.00	63.86	C
ATOM	3818	C	LEU	C	200	43.529	121.093	61.117	1.00	90.93	C
ATOM	3819	O	LEU	C	200	42.614	120.543	60.511	1.00	90.93	C
ATOM	3820	N	TYR	C	201	43.308	122.098	61.954	1.00	78.12	C
ATOM	3821	CA	TYR	C	201	41.939	122.541	62.155	1.00	78.12	C
ATOM	3822	CB	TYR	C	201	41.784	123.185	63.559	1.00	76.20	C
ATOM	3823	CG	TYR	C	201	41.961	124.683	63.682	1.00	76.20	C
ATOM	3824	CD1	TYR	C	201	40.894	125.550	63.453	1.00	76.20	C
ATOM	3825	CE1	TYR	C	201	41.042	126.927	63.581	1.00	76.20	C
ATOM	3826	CD2	TYR	C	201	43.187	125.235	64.044	1.00	76.20	C
ATOM	3827	CE2	TYR	C	201	43.347	126.615	64.173	1.00	76.20	C
ATOM	3828	CZ	TYR	C	201	42.269	127.456	63.940	1.00	76.20	C
ATOM	3829	OH	TYR	C	201	42.404	128.825	64.061	1.00	76.20	C
ATOM	3830	C	TYR	C	201	41.461	123.425	60.988	1.00	78.12	C
ATOM	3831	O	TYR	C	201	41.658	124.641	60.935	1.00	78.12	C
ATOM	3832	N	LYS	C	202	40.879	122.738	60.012	1.00	100.00	C
ATOM	3833	CA	LYS	C	202	40.330	123.334	58.801	1.00	100.00	C
ATOM	3834	CB	LYS	C	202	41.296	123.177	57.628	1.00	86.46	C
ATOM	3835	CG	LYS	C	202	41.577	121.728	57.235	1.00	86.46	C
ATOM	3836	CD	LYS	C	202	42.359	121.645	55.927	1.00	86.46	C
ATOM	3837	CE	LYS	C	202	43.677	122.416	55.990	1.00	86.46	C
ATOM	3838	NZ	LYS	C	202	44.631	121.864	56.998	1.00	86.46	C
ATOM	3839	C	LYS	C	202	39.084	122.503	58.549	1.00	100.00	C
ATOM	3840	O	LYS	C	202	38.406	122.641	57.532	1.00	100.00	C
ATOM	3841	N	ASP	C	203	38.817	121.616	59.500	1.00	97.06	C
ATOM	3842	CA	ASP	C	203	37.659	120.741	59.465	1.00	97.06	C
ATOM	3843	CB	ASP	C	203	38.054	119.328	59.878	1.00	99.98	C

FIGURE 2 Continued

ATOM	3844	CG	ASP	C	203	38.808	119.300	61.187	1.00	99.98	C
ATOM	3845	OD1	ASP	C	203	39.982	119.731	61.211	1.00	99.98	C
ATOM	3846	OD2	ASP	C	203	38.221	118.857	62.193	1.00	99.98	C
ATOM	3847	C	ASP	C	203	36.627	121.297	60.441	1.00	97.06	C
ATOM	3848	O	ASP	C	203	35.569	120.701	60.654	1.00	97.06	C
ATOM	3849	N	ILE	C	204	36.952	122.438	61.046	1.00	67.87	C
ATOM	3850	CA	ILE	C	204	36.032	123.085	61.972	1.00	67.87	C
ATOM	3851	CB	ILE	C	204	36.773	123.813	63.114	1.00	79.05	C
ATOM	3852	CG2	ILE	C	204	35.774	124.321	64.126	1.00	79.05	C
ATOM	3853	CG1	ILE	C	204	37.704	122.852	63.848	1.00	79.05	C
ATOM	3854	CD1	ILE	C	204	38.327	123.463	65.077	1.00	79.05	C
ATOM	3855	C	ILE	C	204	35.177	124.096	61.196	1.00	67.87	C
ATOM	3856	O	ILE	C	204	35.659	124.752	60.274	1.00	67.87	C
ATOM	3857	N	LEU	C	205	33.911	124.208	61.589	1.00	95.77	C
ATOM	3858	CA	LEU	C	205	32.932	125.092	60.951	1.00	95.77	C
ATOM	3859	CB	LEU	C	205	31.664	125.151	61.819	1.00	100.00	C
ATOM	3860	CG	LEU	C	205	31.021	123.821	62.249	1.00	100.00	C
ATOM	3861	CD1	LEU	C	205	29.889	124.093	63.234	1.00	100.00	C
ATOM	3862	CD2	LEU	C	205	30.504	123.064	61.026	1.00	100.00	C
ATOM	3863	C	LEU	C	205	33.366	126.522	60.601	1.00	95.77	C
ATOM	3864	O	LEU	C	205	32.652	127.219	59.882	1.00	95.77	C
ATOM	3865	N	SER	C	206	34.516	126.963	61.107	1.00	75.84	C
ATOM	3866	CA	SER	C	206	35.027	128.317	60.840	1.00	75.84	C
ATOM	3867	CB	SER	C	206	35.253	128.534	59.342	1.00	58.82	C
ATOM	3868	OG	SER	C	206	35.564	129.900	59.083	1.00	58.82	C
ATOM	3869	C	SER	C	206	34.177	129.482	61.354	1.00	75.84	C
ATOM	3870	O	SER	C	206	32.952	129.526	61.076	1.00	75.84	C
ATOM	3871	OXT	SER	C	206	34.777	130.366	62.007	1.00	52.10	C
ATOM	3872	CB	PRO	D	49	66.824	78.431	-12.855	1.00	84.09	D
ATOM	3873	CG	PRO	D	49	65.930	77.235	-12.554	1.00	84.09	D
ATOM	3874	C	PRO	D	49	67.642	79.232	-10.616	1.00	84.09	D
ATOM	3875	O	PRO	D	49	68.213	80.320	-10.542	1.00	84.09	D
ATOM	3876	N	PRO	D	49	67.924	76.869	-11.366	1.00	84.09	D
ATOM	3877	CD	PRO	D	49	66.891	76.118	-12.101	1.00	84.09	D
ATOM	3878	CA	PRO	D	49	67.905	78.289	-11.787	1.00	84.09	D
ATOM	3879	N	ALA	D	50	66.771	78.819	-9.704	1.00	75.27	D
ATOM	3880	CA	ALA	D	50	66.463	79.643	-8.546	1.00	75.27	D
ATOM	3881	CB	ALA	D	50	65.119	79.243	-7.964	1.00	100.00	D
ATOM	3882	C	ALA	D	50	67.571	79.446	-7.515	1.00	75.27	D
ATOM	3883	O	ALA	D	50	68.080	80.413	-6.941	1.00	75.27	D
ATOM	3884	N	VAL	D	51	67.944	78.187	-7.290	1.00	72.18	D
ATOM	3885	CA	VAL	D	51	68.996	77.858	-6.337	1.00	72.18	D
ATOM	3886	CB	VAL	D	51	69.176	76.325	-6.184	1.00	58.48	D
ATOM	3887	CG1	VAL	D	51	70.457	76.024	-5.407	1.00	58.48	D
ATOM	3888	CG2	VAL	D	51	67.987	75.729	-5.451	1.00	58.48	D
ATOM	3889	C	VAL	D	51	70.321	78.450	-6.789	1.00	72.18	D
ATOM	3890	O	VAL	D	51	71.118	78.900	-5.965	1.00	72.18	D
ATOM	3891	N	THR	D	52	70.548	78.449	-8.100	1.00	62.28	D
ATOM	3892	CA	THR	D	52	71.785	78.976	-8.666	1.00	62.28	D
ATOM	3893	CB	THR	D	52	71.877	78.690	-10.188	1.00	100.00	D
ATOM	3894	OG1	THR	D	52	73.163	79.091	-10.675	1.00	100.00	D
ATOM	3895	CG2	THR	D	52	70.811	79.452	-10.947	1.00	100.00	D
ATOM	3896	C	THR	D	52	71.911	80.478	-8.420	1.00	62.28	D
ATOM	3897	O	THR	D	52	72.986	80.972	-8.088	1.00	62.28	D
ATOM	3898	N	ASP	D	53	70.811	81.203	-8.583	1.00	58.35	D
ATOM	3899	CA	ASP	D	53	70.831	82.634	-8.348	1.00	58.35	D
ATOM	3900	CB	ASP	D	53	69.556	83.277	-8.886	1.00	100.00	D

FIGURE 2 Continued

ATOM	3901	CG	ASP	D	53	69.555	83.376	-10.397	1.00	100.00	D
ATOM	3902	OD1	ASP	D	53	69.761	82.339	-11.062	1.00	100.00	D
ATOM	3903	OD2	ASP	D	53	69.350	84.492	-10.918	1.00	100.00	D
ATOM	3904	C	ASP	D	53	70.980	82.902	-6.853	1.00	58.35	D
ATOM	3905	O	ASP	D	53	71.590	83.892	-6.446	1.00	58.35	D
ATOM	3906	N	LEU	D	54	70.434	82.007	-6.036	1.00	51.66	D
ATOM	3907	CA	LEU	D	54	70.534	82.152	-4.595	1.00	51.66	D
ATOM	3908	CB	LEU	D	54	69.611	81.159	-3.896	1.00	43.71	D
ATOM	3909	CG	LEU	D	54	69.558	81.287	-2.371	1.00	43.71	D
ATOM	3910	CD1	LEU	D	54	69.054	82.685	-2.001	1.00	43.71	D
ATOM	3911	CD2	LEU	D	54	68.656	80.205	-1.787	1.00	43.71	D
ATOM	3912	C	LEU	D	54	71.977	81.917	-4.165	1.00	51.66	D
ATOM	3913	O	LEU	D	54	72.528	82.677	-3.370	1.00	51.66	D
ATOM	3914	N	ASP	D	55	72.601	80.872	-4.693	1.00	58.79	D
ATOM	3915	CA	ASP	D	55	73.982	80.600	-4.329	1.00	58.79	D
ATOM	3916	CB	ASP	D	55	74.441	79.251	-4.874	1.00	70.83	D
ATOM	3917	CG	ASP	D	55	73.811	78.096	-4.137	1.00	70.83	D
ATOM	3918	OD1	ASP	D	55	73.639	78.211	-2.903	1.00	70.83	D
ATOM	3919	OD2	ASP	D	55	73.497	77.074	-4.784	1.00	70.83	D
ATOM	3920	C	ASP	D	55	74.891	81.698	-4.835	1.00	58.79	D
ATOM	3921	O	ASP	D	55	75.857	82.060	-4.170	1.00	58.79	D
ATOM	3922	N	HIS	D	56	74.582	82.232	-6.010	1.00	59.43	D
ATOM	3923	CA	HIS	D	56	75.383	83.311	-6.570	1.00	59.43	D
ATOM	3924	CB	HIS	D	56	74.833	83.731	-7.936	1.00	91.91	D
ATOM	3925	CG	HIS	D	56	75.533	84.914	-8.532	1.00	91.91	D
ATOM	3926	CD2	HIS	D	56	75.068	86.132	-8.902	1.00	91.91	D
ATOM	3927	ND1	HIS	D	56	76.884	84.921	-8.805	1.00	91.91	D
ATOM	3928	CE1	HIS	D	56	77.222	86.092	-9.318	1.00	91.91	D
ATOM	3929	NE2	HIS	D	56	76.139	86.845	-9.388	1.00	91.91	D
ATOM	3930	C	HIS	D	56	75.323	84.492	-5.603	1.00	59.43	D
ATOM	3931	O	HIS	D	56	76.330	85.145	-5.318	1.00	59.43	D
ATOM	3932	N	LEU	D	57	74.130	84.744	-5.081	1.00	47.08	D
ATOM	3933	CA	LEU	D	57	73.933	85.845	-4.161	1.00	47.08	D
ATOM	3934	CB	LEU	D	57	72.434	86.065	-3.938	1.00	61.70	D
ATOM	3935	CG	LEU	D	57	72.000	87.364	-3.261	1.00	61.70	D
ATOM	3936	CD1	LEU	D	57	72.801	88.541	-3.788	1.00	61.70	D
ATOM	3937	CD2	LEU	D	57	70.525	87.567	-3.517	1.00	61.70	D
ATOM	3938	C	LEU	D	57	74.652	85.593	-2.838	1.00	47.08	D
ATOM	3939	O	LEU	D	57	75.218	86.518	-2.247	1.00	47.08	D
ATOM	3940	N	LYS	D	58	74.643	84.341	-2.382	1.00	31.13	D
ATOM	3941	CA	LYS	D	58	75.309	83.998	-1.134	1.00	31.13	D
ATOM	3942	CB	LYS	D	58	75.046	82.538	-0.777	1.00	35.52	D
ATOM	3943	CG	LYS	D	58	73.614	82.288	-0.322	1.00	35.52	D
ATOM	3944	CD	LYS	D	58	73.443	80.883	0.205	1.00	35.52	D
ATOM	3945	CE	LYS	D	58	72.066	80.705	0.788	1.00	35.52	D
ATOM	3946	NZ	LYS	D	58	71.923	79.393	1.458	1.00	35.52	D
ATOM	3947	C	LYS	D	58	76.808	84.263	-1.238	1.00	31.13	D
ATOM	3948	O	LYS	D	58	77.445	84.706	-0.265	1.00	31.13	D
ATOM	3949	N	GLY	D	59	77.354	84.004	-2.430	1.00	38.25	D
ATOM	3950	CA	GLY	D	59	78.765	84.225	-2.684	1.00	38.25	D
ATOM	3951	C	GLY	D	59	79.093	85.704	-2.610	1.00	38.25	D
ATOM	3952	O	GLY	D	59	80.106	86.087	-2.018	1.00	38.25	D
ATOM	3953	N	ILE	D	60	78.243	86.534	-3.218	1.00	35.08	D
ATOM	3954	CA	ILE	D	60	78.433	87.987	-3.182	1.00	35.08	D
ATOM	3955	CB	ILE	D	60	77.232	88.763	-3.806	1.00	40.77	D
ATOM	3956	CG2	ILE	D	60	77.513	90.256	-3.771	1.00	40.77	D
ATOM	3957	CG1	ILE	D	60	76.946	88.280	-5.239	1.00	40.77	D

FIGURE 2 Continued

ATOM	3958	CD1	ILE	D	60	78.061	88.489	-6.226	1.00	40.77	D
ATOM	3959	C	ILE	D	60	78.497	88.375	-1.703	1.00	35.08	D
ATOM	3960	O	ILE	D	60	79.406	89.079	-1.261	1.00	35.08	D
ATOM	3961	N	LEU	D	61	77.522	87.896	-0.938	1.00	37.37	D
ATOM	3962	CA	LEU	D	61	77.452	88.200	0.485	1.00	37.37	D
ATOM	3963	CB	LEU	D	61	76.125	87.713	1.071	1.00	42.70	D
ATOM	3964	CG	LEU	D	61	74.921	88.664	1.029	1.00	42.70	D
ATOM	3965	CD1	LEU	D	61	74.498	88.975	-0.404	1.00	42.70	D
ATOM	3966	CD2	LEU	D	61	73.776	88.006	1.784	1.00	42.70	D
ATOM	3967	C	LEU	D	61	78.606	87.629	1.304	1.00	37.37	D
ATOM	3968	O	LEU	D	61	78.756	87.975	2.467	1.00	37.37	D
ATOM	3969	N	ARG	D	62	79.410	86.747	0.712	1.00	36.92	D
ATOM	3970	CA	ARG	D	62	80.538	86.183	1.446	1.00	36.92	D
ATOM	3971	CB	ARG	D	62	80.653	84.666	1.228	1.00	56.32	D
ATOM	3972	CG	ARG	D	62	79.572	83.838	1.930	1.00	56.32	D
ATOM	3973	CD	ARG	D	62	79.863	82.348	1.825	1.00	56.32	D
ATOM	3974	NE	ARG	D	62	78.653	81.562	1.577	1.00	56.32	D
ATOM	3975	CZ	ARG	D	62	77.859	81.063	2.523	1.00	56.32	D
ATOM	3976	NH1	ARG	D	62	78.135	81.252	3.807	1.00	56.32	D
ATOM	3977	NH2	ARG	D	62	76.776	80.379	2.180	1.00	56.32	D
ATOM	3978	C	ARG	D	62	81.822	86.889	1.028	1.00	36.92	D
ATOM	3979	O	ARG	D	62	82.926	86.392	1.244	1.00	36.92	D
ATOM	3980	N	ARG	D	63	81.670	88.059	0.423	1.00	37.56	D
ATOM	3981	CA	ARG	D	63	82.831	88.828	0.018	1.00	37.56	D
ATOM	3982	CB	ARG	D	63	82.446	89.891	-0.999	1.00	47.92	D
ATOM	3983	CG	ARG	D	63	82.249	89.273	-2.359	1.00	47.92	D
ATOM	3984	CD	ARG	D	63	81.915	90.272	-3.415	1.00	47.92	D
ATOM	3985	NE	ARG	D	63	81.769	89.602	-4.700	1.00	47.92	D
ATOM	3986	CZ	ARG	D	63	81.385	90.209	-5.817	1.00	47.92	D
ATOM	3987	NH1	ARG	D	63	81.108	91.510	-5.798	1.00	47.92	D
ATOM	3988	NH2	ARG	D	63	81.278	89.512	-6.944	1.00	47.92	D
ATOM	3989	C	ARG	D	63	83.408	89.423	1.281	1.00	37.56	D
ATOM	3990	O	ARG	D	63	82.691	89.941	2.140	1.00	37.56	D
ATOM	3991	N	ARG	D	64	84.719	89.349	1.392	1.00	33.60	D
ATOM	3992	CA	ARG	D	64	85.368	89.786	2.598	1.00	33.60	D
ATOM	3993	CB	ARG	D	64	85.493	88.551	3.508	1.00	37.75	D
ATOM	3994	CG	ARG	D	64	85.167	88.749	4.971	1.00	37.75	D
ATOM	3995	CD	ARG	D	64	83.926	87.968	5.397	1.00	37.75	D
ATOM	3996	NE	ARG	D	64	82.798	88.345	4.571	1.00	37.75	D
ATOM	3997	CZ	ARG	D	64	81.547	87.936	4.739	1.00	37.75	D
ATOM	3998	NH1	ARG	D	64	81.219	87.109	5.722	1.00	37.75	D
ATOM	3999	NH2	ARG	D	64	80.621	88.379	3.905	1.00	37.75	D
ATOM	4000	C	ARG	D	64	86.755	90.353	2.300	1.00	33.60	D
ATOM	4001	O	ARG	D	64	87.267	90.248	1.183	1.00	33.60	D
ATOM	4002	N	GLN	D	65	87.338	90.986	3.308	1.00	37.58	D
ATOM	4003	CA	GLN	D	65	88.696	91.486	3.222	1.00	37.58	D
ATOM	4004	CB	GLN	D	65	88.776	92.985	3.470	1.00	44.35	D
ATOM	4005	CG	GLN	D	65	88.206	93.845	2.369	1.00	44.35	D
ATOM	4006	CD	GLN	D	65	88.575	95.308	2.551	1.00	44.35	D
ATOM	4007	OE1	GLN	D	65	89.723	95.705	2.325	1.00	44.35	D
ATOM	4008	NE2	GLN	D	65	87.604	96.115	2.982	1.00	44.35	D
ATOM	4009	C	GLN	D	65	89.295	90.733	4.405	1.00	37.58	D
ATOM	4010	O	GLN	D	65	88.663	90.620	5.449	1.00	37.58	D
ATOM	4011	N	LEU	D	66	90.488	90.189	4.248	1.00	36.57	D
ATOM	4012	CA	LEU	D	66	91.088	89.449	5.330	1.00	36.57	D
ATOM	4013	CB	LEU	D	66	91.546	88.087	4.819	1.00	36.18	D
ATOM	4014	CG	LEU	D	66	91.676	86.992	5.871	1.00	36.18	D

FIGURE 2 Continued

ATOM	4015	CD1	LEU	D	66	90.363	86.847	6.657	1.00	36.18	D
ATOM	4016	CD2	LEU	D	66	92.040	85.684	5.168	1.00	36.18	D
ATOM	4017	C	LEU	D	66	92.245	90.269	5.869	1.00	36.57	D
ATOM	4018	O	LEU	D	66	93.322	90.330	5.275	1.00	36.57	D
ATOM	4019	N	TYR	D	67	92.002	90.904	7.008	1.00	33.90	D
ATOM	4020	CA	TYR	D	67	92.981	91.767	7.638	1.00	33.90	D
ATOM	4021	CB	TYR	D	67	92.248	92.923	8.327	1.00	38.66	D
ATOM	4022	CG	TYR	D	67	93.134	93.857	9.126	1.00	38.66	D
ATOM	4023	CD1	TYR	D	67	94.012	94.740	8.491	1.00	38.66	D
ATOM	4024	CE1	TYR	D	67	94.815	95.599	9.223	1.00	38.66	D
ATOM	4025	CD2	TYR	D	67	93.089	93.861	10.520	1.00	38.66	D
ATOM	4026	CE2	TYR	D	67	93.890	94.717	11.262	1.00	38.66	D
ATOM	4027	CZ	TYR	D	67	94.751	95.584	10.605	1.00	38.66	D
ATOM	4028	OH	TYR	D	67	95.551	96.428	11.343	1.00	38.66	D
ATOM	4029	C	TYR	D	67	93.878	91.045	8.635	1.00	33.90	D
ATOM	4030	O	TYR	D	67	93.406	90.487	9.621	1.00	33.90	D
ATOM	4031	N	CYS	D	68	95.179	91.059	8.370	1.00	34.51	D
ATOM	4032	CA	CYS	D	68	96.136	90.425	9.265	1.00	34.51	D
ATOM	4033	CB	CYS	D	68	97.427	90.090	8.510	1.00	38.62	D
ATOM	4034	SG	CYS	D	68	98.499	88.931	9.390	1.00	38.62	D
ATOM	4035	C	CYS	D	68	96.422	91.424	10.388	1.00	34.51	D
ATOM	4036	O	CYS	D	68	96.511	92.625	10.134	1.00	34.51	D
ATOM	4037	N	ARG	D	69	96.546	90.935	11.622	1.00	43.41	D
ATOM	4038	CA	ARG	D	69	96.802	91.813	12.760	1.00	43.41	D
ATOM	4039	CB	ARG	D	69	96.841	91.015	14.067	1.00	65.33	D
ATOM	4040	CG	ARG	D	69	96.942	91.902	15.298	1.00	65.33	D
ATOM	4041	CD	ARG	D	69	96.692	91.136	16.583	1.00	65.33	D
ATOM	4042	NE	ARG	D	69	96.974	91.958	17.763	1.00	65.33	D
ATOM	4043	CZ	ARG	D	69	96.797	91.559	19.023	1.00	65.33	D
ATOM	4044	NH1	ARG	D	69	96.333	90.342	19.277	1.00	65.33	D
ATOM	4045	NH2	ARG	D	69	97.089	92.376	20.028	1.00	65.33	D
ATOM	4046	C	ARG	D	69	98.124	92.533	12.546	1.00	43.41	D
ATOM	4047	O	ARG	D	69	98.451	93.515	13.209	1.00	43.41	D
ATOM	4048	N	THR	D	70	98.872	92.035	11.582	1.00	50.64	D
ATOM	4049	CA	THR	D	70	100.158	92.588	11.250	1.00	50.64	D
ATOM	4050	CB	THR	D	70	100.893	91.563	10.355	1.00	43.03	D
ATOM	4051	OG1	THR	D	70	102.225	91.376	10.840	1.00	43.03	D
ATOM	4052	CG2	THR	D	70	100.895	91.979	8.924	1.00	43.03	D
ATOM	4053	C	THR	D	70	99.973	93.965	10.588	1.00	50.64	D
ATOM	4054	O	THR	D	70	100.930	94.715	10.401	1.00	50.64	D
ATOM	4055	N	GLY	D	71	98.726	94.300	10.261	1.00	38.67	D
ATOM	4056	CA	GLY	D	71	98.429	95.581	9.648	1.00	38.67	D
ATOM	4057	C	GLY	D	71	98.105	95.522	8.169	1.00	38.67	D
ATOM	4058	O	GLY	D	71	97.850	96.552	7.550	1.00	38.67	D
ATOM	4059	N	PHE	D	72	98.094	94.328	7.588	1.00	35.55	D
ATOM	4060	CA	PHE	D	72	97.824	94.214	6.159	1.00	35.55	D
ATOM	4061	CB	PHE	D	72	99.078	93.733	5.406	1.00	38.85	D
ATOM	4062	CG	PHE	D	72	100.327	94.508	5.724	1.00	38.85	D
ATOM	4063	CD1	PHE	D	72	101.051	94.241	6.875	1.00	38.85	D
ATOM	4064	CD2	PHE	D	72	100.786	95.507	4.861	1.00	38.85	D
ATOM	4065	CE1	PHE	D	72	102.221	94.957	7.176	1.00	38.85	D
ATOM	4066	CE2	PHE	D	72	101.957	96.233	5.148	1.00	38.85	D
ATOM	4067	CZ	PHE	D	72	102.674	95.955	6.307	1.00	38.85	D
ATOM	4068	C	PHE	D	72	96.680	93.292	5.763	1.00	35.55	D
ATOM	4069	O	PHE	D	72	96.394	92.294	6.430	1.00	35.55	D
ATOM	4070	N	HIS	D	73	96.048	93.637	4.648	1.00	40.58	D
ATOM	4071	CA	HIS	D	73	94.976	92.845	4.076	1.00	40.58	D

FIGURE 2 Continued

ATOM	4072	CB	HIS	D	73	93.993	93.733	3.317	1.00	48.44	D
ATOM	4073	CG	HIS	D	73	93.149	94.596	4.198	1.00	48.44	D
ATOM	4074	CD2	HIS	D	73	92.081	94.299	4.974	1.00	48.44	D
ATOM	4075	ND1	HIS	D	73	93.359	95.949	4.337	1.00	48.44	D
ATOM	4076	CE1	HIS	D	73	92.455	96.452	5.158	1.00	48.44	D
ATOM	4077	NE2	HIS	D	73	91.668	95.471	5.559	1.00	48.44	D
ATOM	4078	C	HIS	D	73	95.622	91.876	3.090	1.00	40.58	D
ATOM	4079	O	HIS	D	73	96.547	92.243	2.377	1.00	40.58	D
ATOM	4080	N	LEU	D	74	95.141	90.644	3.035	1.00	39.53	D
ATOM	4081	CA	LEU	D	74	95.714	89.684	2.112	1.00	39.53	D
ATOM	4082	CB	LEU	D	74	95.354	88.267	2.538	1.00	38.15	D
ATOM	4083	CG	LEU	D	74	96.038	87.167	1.732	1.00	38.15	D
ATOM	4084	CD1	LEU	D	74	96.466	86.054	2.669	1.00	38.15	D
ATOM	4085	CD2	LEU	D	74	95.099	86.659	0.641	1.00	38.15	D
ATOM	4086	C	LEU	D	74	95.222	89.950	0.694	1.00	39.53	D
ATOM	4087	O	LEU	D	74	94.045	90.230	0.473	1.00	39.53	D
ATOM	4088	N	GLU	D	75	96.140	89.867	-0.268	1.00	44.34	D
ATOM	4089	CA	GLU	D	75	95.822	90.099	-1.667	1.00	44.34	D
ATOM	4090	CB	GLU	D	75	96.595	91.302	-2.189	1.00	46.41	D
ATOM	4091	CG	GLU	D	75	96.105	92.631	-1.694	1.00	46.41	D
ATOM	4092	CD	GLU	D	75	97.019	93.751	-2.106	1.00	46.41	D
ATOM	4093	OE1	GLU	D	75	98.156	93.785	-1.592	1.00	46.41	D
ATOM	4094	OE2	GLU	D	75	96.604	94.588	-2.937	1.00	46.41	D
ATOM	4095	C	GLU	D	75	96.187	88.914	-2.517	1.00	44.34	D
ATOM	4096	O	GLU	D	75	97.176	88.240	-2.263	1.00	44.34	D
ATOM	4097	N	ILE	D	76	95.394	88.665	-3.546	1.00	35.83	D
ATOM	4098	CA	ILE	D	76	95.678	87.565	-4.461	1.00	35.83	D
ATOM	4099	CB	ILE	D	76	94.551	86.524	-4.443	1.00	39.96	D
ATOM	4100	CG2	ILE	D	76	94.878	85.401	-5.409	1.00	39.96	D
ATOM	4101	CG1	ILE	D	76	94.361	86.005	-3.011	1.00	39.96	D
ATOM	4102	CD1	ILE	D	76	93.289	84.948	-2.848	1.00	39.96	D
ATOM	4103	C	ILE	D	76	95.815	88.152	-5.864	1.00	35.83	D
ATOM	4104	O	ILE	D	76	94.817	88.476	-6.509	1.00	35.83	D
ATOM	4105	N	PHE	D	77	97.053	88.304	-6.329	1.00	43.90	D
ATOM	4106	CA	PHE	D	77	97.292	88.877	-7.649	1.00	43.90	D
ATOM	4107	CB	PHE	D	77	98.687	89.486	-7.714	1.00	46.13	D
ATOM	4108	CG	PHE	D	77	98.816	90.749	-6.924	1.00	46.13	D
ATOM	4109	CD1	PHE	D	77	99.148	90.714	-5.574	1.00	46.13	D
ATOM	4110	CD2	PHE	D	77	98.536	91.985	-7.514	1.00	46.13	D
ATOM	4111	CE1	PHE	D	77	99.198	91.891	-4.824	1.00	46.13	D
ATOM	4112	CE2	PHE	D	77	98.585	93.172	-6.765	1.00	46.13	D
ATOM	4113	CZ	PHE	D	77	98.915	93.123	-5.422	1.00	46.13	D
ATOM	4114	C	PHE	D	77	97.080	87.922	-8.814	1.00	43.90	D
ATOM	4115	O	PHE	D	77	97.268	86.712	-8.688	1.00	43.90	D
ATOM	4116	N	PRO	D	78	96.661	88.465	-9.969	1.00	52.17	D
ATOM	4117	CD	PRO	D	78	96.356	89.893	-10.193	1.00	38.51	D
ATOM	4118	CA	PRO	D	78	96.412	87.678	-11.182	1.00	52.17	D
ATOM	4119	CB	PRO	D	78	96.156	88.742	-12.242	1.00	38.51	D
ATOM	4120	CG	PRO	D	78	95.522	89.850	-11.456	1.00	38.51	D
ATOM	4121	C	PRO	D	78	97.570	86.763	-11.555	1.00	52.17	D
ATOM	4122	O	PRO	D	78	97.351	85.695	-12.122	1.00	52.17	D
ATOM	4123	N	ASN	D	79	98.798	87.169	-11.240	1.00	51.23	D
ATOM	4124	CA	ASN	D	79	99.946	86.337	-11.569	1.00	51.23	D
ATOM	4125	CB	ASN	D	79	101.202	87.189	-11.839	1.00	61.00	D
ATOM	4126	CG	ASN	D	79	101.710	87.950	-10.619	1.00	61.00	D
ATOM	4127	OD1	ASN	D	79	101.277	87.744	-9.486	1.00	61.00	D
ATOM	4128	ND2	ASN	D	79	102.679	88.824	-10.890	1.00	61.00	D

FIGURE 2 Continued

ATOM	4129	C	ASN	D	79	100.245	85.245	-10.540	1.00	51.23	D
ATOM	4130	O	ASN	D	79	101.346	84.690	-10.517	1.00	51.23	D
ATOM	4131	N	GLY	D	80	99.253	84.930	-9.706	1.00	38.19	D
ATOM	4132	CA	GLY	D	80	99.413	83.884	-8.702	1.00	38.19	D
ATOM	4133	C	GLY	D	80	100.249	84.266	-7.495	1.00	38.19	D
ATOM	4134	O	GLY	D	80	100.559	83.436	-6.654	1.00	38.19	D
ATOM	4135	N	THR	D	81	100.615	85.534	-7.411	1.00	47.14	D
ATOM	4136	CA	THR	D	81	101.423	86.022	-6.305	1.00	47.14	D
ATOM	4137	CB	THR	D	81	102.348	87.173	-6.808	1.00	57.15	D
ATOM	4138	OG1	THR	D	81	103.588	86.604	-7.251	1.00	57.15	D
ATOM	4139	CG2	THR	D	81	102.606	88.211	-5.733	1.00	57.15	D
ATOM	4140	C	THR	D	81	100.543	86.485	-5.139	1.00	47.14	D
ATOM	4141	O	THR	D	81	99.392	86.881	-5.342	1.00	47.14	D
ATOM	4142	N	ILE	D	82	101.085	86.406	-3.921	1.00	44.74	D
ATOM	4143	CA	ILE	D	82	100.369	86.832	-2.725	1.00	44.74	D
ATOM	4144	CB	ILE	D	82	100.098	85.657	-1.745	1.00	33.10	D
ATOM	4145	CG2	ILE	D	82	99.292	86.165	-0.543	1.00	33.10	D
ATOM	4146	CG1	ILE	D	82	99.319	84.537	-2.435	1.00	33.10	D
ATOM	4147	CD1	ILE	D	82	97.988	84.971	-2.969	1.00	33.10	D
ATOM	4148	C	ILE	D	82	101.174	87.870	-1.952	1.00	44.74	D
ATOM	4149	O	ILE	D	82	102.397	87.768	-1.844	1.00	44.74	D
ATOM	4150	N	GLN	D	83	100.483	88.871	-1.416	1.00	53.73	D
ATOM	4151	CA	GLN	D	83	101.126	89.898	-0.608	1.00	53.73	D
ATOM	4152	CB	GLN	D	83	101.964	90.843	-1.469	1.00	70.07	D
ATOM	4153	CG	GLN	D	83	101.219	91.534	-2.574	1.00	70.07	D
ATOM	4154	CD	GLN	D	83	102.132	92.400	-3.422	1.00	70.07	D
ATOM	4155	OE1	GLN	D	83	102.690	93.382	-2.944	1.00	70.07	D
ATOM	4156	NE2	GLN	D	83	102.294	92.031	-4.687	1.00	70.07	D
ATOM	4157	C	GLN	D	83	100.074	90.675	0.162	1.00	53.73	D
ATOM	4158	O	GLN	D	83	98.876	90.511	-0.074	1.00	53.73	D
ATOM	4159	N	GLY	D	84	100.520	91.506	1.096	1.00	56.43	D
ATOM	4160	CA	GLY	D	84	99.587	92.273	1.889	1.00	56.43	D
ATOM	4161	C	GLY	D	84	99.651	93.750	1.591	1.00	56.43	D
ATOM	4162	O	GLY	D	84	100.669	94.251	1.112	1.00	56.43	D
ATOM	4163	N	THR	D	85	98.559	94.450	1.878	1.00	50.58	D
ATOM	4164	CA	THR	D	85	98.487	95.882	1.650	1.00	50.58	D
ATOM	4165	CB	THR	D	85	97.791	96.202	0.330	1.00	42.66	D
ATOM	4166	OG1	THR	D	85	97.776	97.619	0.142	1.00	42.66	D
ATOM	4167	CG2	THR	D	85	96.365	95.688	0.339	1.00	42.66	D
ATOM	4168	C	THR	D	85	97.728	96.577	2.768	1.00	50.58	D
ATOM	4169	O	THR	D	85	96.665	96.120	3.192	1.00	50.58	D
ATOM	4170	N	ARG	D	86	98.282	97.687	3.243	1.00	43.79	D
ATOM	4171	CA	ARG	D	86	97.656	98.460	4.306	1.00	43.79	D
ATOM	4172	CB	ARG	D	86	98.632	99.519	4.828	1.00	62.75	D
ATOM	4173	CG	ARG	D	86	99.804	98.948	5.612	1.00	62.75	D
ATOM	4174	CD	ARG	D	86	100.765	100.040	6.061	1.00	62.75	D
ATOM	4175	NE	ARG	D	86	101.803	99.554	6.974	1.00	62.75	D
ATOM	4176	CZ	ARG	D	86	101.578	99.111	8.213	1.00	62.75	D
ATOM	4177	NH1	ARG	D	86	100.340	99.086	8.701	1.00	62.75	D
ATOM	4178	NH2	ARG	D	86	102.593	98.703	8.972	1.00	62.75	D
ATOM	4179	C	ARG	D	86	96.376	99.118	3.792	1.00	43.79	D
ATOM	4180	O	ARG	D	86	95.472	99.417	4.563	1.00	43.79	D
ATOM	4181	N	LYS	D	87	96.297	99.321	2.481	1.00	53.52	D
ATOM	4182	CA	LYS	D	87	95.130	99.953	1.874	1.00	53.52	D
ATOM	4183	CB	LYS	D	87	95.336	100.094	0.366	1.00	77.32	D
ATOM	4184	CG	LYS	D	87	96.521	100.978	0.027	1.00	77.32	D
ATOM	4185	CD	LYS	D	87	96.897	100.907	-1.439	1.00	77.32	D

FIGURE 2 Continued

ATOM	4186	CE	LYS	D	87	98.142	101.741	-1.712	1.00	77.32	D
ATOM	4187	NZ	LYS	D	87	98.610	101.608	-3.123	1.00	77.32	D
ATOM	4188	C	LYS	D	87	93.846	99.192	2.153	1.00	53.52	D
ATOM	4189	O	LYS	D	87	93.847	97.970	2.307	1.00	53.52	D
ATOM	4190	N	ASP	D	88	92.748	99.929	2.232	1.00	46.76	D
ATOM	4191	CA	ASP	D	88	91.443	99.338	2.482	1.00	46.76	D
ATOM	4192	CB	ASP	D	88	90.643	100.243	3.425	1.00	47.07	D
ATOM	4193	CG	ASP	D	88	89.224	99.757	3.653	1.00	47.07	D
ATOM	4194	OD1	ASP	D	88	89.030	98.551	3.909	1.00	47.07	D
ATOM	4195	OD2	ASP	D	88	88.296	100.592	3.591	1.00	47.07	D
ATOM	4196	C	ASP	D	88	90.746	99.197	1.138	1.00	46.76	D
ATOM	4197	O	ASP	D	88	90.877	100.058	0.270	1.00	46.76	D
ATOM	4198	N	HIS	D	89	90.022	98.102	0.956	1.00	43.41	D
ATOM	4199	CA	HIS	D	89	89.318	97.870	-0.299	1.00	43.41	D
ATOM	4200	CB	HIS	D	89	88.199	98.897	-0.482	1.00	46.70	D
ATOM	4201	CG	HIS	D	89	86.993	98.617	0.353	1.00	46.70	D
ATOM	4202	CD2	HIS	D	89	85.845	97.958	0.064	1.00	46.70	D
ATOM	4203	ND1	HIS	D	89	86.907	98.978	1.679	1.00	46.70	D
ATOM	4204	CE1	HIS	D	89	85.757	98.552	2.172	1.00	46.70	D
ATOM	4205	NE2	HIS	D	89	85.095	97.930	1.213	1.00	46.70	D
ATOM	4206	C	HIS	D	89	90.212	97.877	-1.540	1.00	43.41	D
ATOM	4207	O	HIS	D	89	89.816	98.393	-2.591	1.00	43.41	D
ATOM	4208	N	SER	D	90	91.408	97.304	-1.425	1.00	47.53	D
ATOM	4209	CA	SER	D	90	92.313	97.247	-2.566	1.00	47.53	D
ATOM	4210	CB	SER	D	90	93.697	96.786	-2.137	1.00	54.51	D
ATOM	4211	OG	SER	D	90	93.686	95.404	-1.860	1.00	54.51	D
ATOM	4212	C	SER	D	90	91.737	96.265	-3.583	1.00	47.53	D
ATOM	4213	O	SER	D	90	91.098	95.282	-3.221	1.00	47.53	D
ATOM	4214	N	ARG	D	91	91.971	96.544	-4.857	1.00	47.05	D
ATOM	4215	CA	ARG	D	91	91.469	95.722	-5.950	1.00	47.05	D
ATOM	4216	CB	ARG	D	91	92.181	96.135	-7.244	1.00	79.19	D
ATOM	4217	CG	ARG	D	91	91.706	95.425	-8.499	1.00	79.19	D
ATOM	4218	CD	ARG	D	91	92.532	95.849	-9.707	1.00	79.19	D
ATOM	4219	NE	ARG	D	91	92.236	95.042	-10.890	1.00	79.19	D
ATOM	4220	CZ	ARG	D	91	92.905	95.123	-12.038	1.00	79.19	D
ATOM	4221	NH1	ARG	D	91	93.912	95.978	-12.162	1.00	79.19	D
ATOM	4222	NH2	ARG	D	91	92.577	94.340	-13.057	1.00	79.19	D
ATOM	4223	C	ARG	D	91	91.601	94.209	-5.735	1.00	47.05	D
ATOM	4224	O	ARG	D	91	90.643	93.459	-5.920	1.00	47.05	D
ATOM	4225	N	PHE	D	92	92.785	93.763	-5.339	1.00	49.96	D
ATOM	4226	CA	PHE	D	92	93.024	92.342	-5.154	1.00	49.96	D
ATOM	4227	CB	PHE	D	92	94.396	91.994	-5.730	1.00	47.04	D
ATOM	4228	CG	PHE	D	92	94.533	92.362	-7.176	1.00	47.04	D
ATOM	4229	CD1	PHE	D	92	93.747	91.732	-8.143	1.00	47.04	D
ATOM	4230	CD2	PHE	D	92	95.392	93.387	-7.573	1.00	47.04	D
ATOM	4231	CE1	PHE	D	92	93.808	92.119	-9.489	1.00	47.04	D
ATOM	4232	CE2	PHE	D	92	95.460	93.781	-8.914	1.00	47.04	D
ATOM	4233	CZ	PHE	D	92	94.662	93.141	-9.873	1.00	47.04	D
ATOM	4234	C	PHE	D	92	92.897	91.881	-3.713	1.00	49.96	D
ATOM	4235	O	PHE	D	92	93.260	90.748	-3.378	1.00	49.96	D
ATOM	4236	N	GLY	D	93	92.368	92.771	-2.875	1.00	44.36	D
ATOM	4237	CA	GLY	D	93	92.157	92.466	-1.473	1.00	44.36	D
ATOM	4238	C	GLY	D	93	90.716	92.045	-1.219	1.00	44.36	D
ATOM	4239	O	GLY	D	93	90.361	91.680	-0.101	1.00	44.36	D
ATOM	4240	N	ILE	D	94	89.882	92.099	-2.255	1.00	47.02	D
ATOM	4241	CA	ILE	D	94	88.482	91.697	-2.141	1.00	47.02	D
ATOM	4242	CB	ILE	D	94	87.600	92.417	-3.177	1.00	39.61	D

FIGURE 2 Continued

ATOM	4243	CG2	ILE	D	94	86.143	92.016	-2.979	1.00	39.61	D
ATOM	4244	CG1	ILE	D	94	87.779	93.931	-3.058	1.00	39.61	D
ATOM	4245	CD1	ILE	D	94	87.448	94.491	-1.682	1.00	39.61	D
ATOM	4246	C	ILE	D	94	88.412	90.193	-2.406	1.00	47.02	D
ATOM	4247	O	ILE	D	94	88.647	89.742	-3.529	1.00	47.02	D
ATOM	4248	N	LEU	D	95	88.073	89.423	-1.375	1.00	44.82	D
ATOM	4249	CA	LEU	D	95	88.019	87.971	-1.488	1.00	44.82	D
ATOM	4250	CB	LEU	D	95	88.994	87.369	-0.481	1.00	31.17	D
ATOM	4251	CG	LEU	D	95	90.243	88.226	-0.213	1.00	31.17	D
ATOM	4252	CD1	LEU	D	95	90.960	87.729	1.029	1.00	31.17	D
ATOM	4253	CD2	LEU	D	95	91.181	88.198	-1.424	1.00	31.17	D
ATOM	4254	C	LEU	D	95	86.629	87.414	-1.225	1.00	44.82	D
ATOM	4255	O	LEU	D	95	85.858	88.003	-0.489	1.00	44.82	D
ATOM	4256	N	GLU	D	96	86.316	86.272	-1.826	1.00	37.43	D
ATOM	4257	CA	GLU	D	96	85.030	85.614	-1.617	1.00	37.43	D
ATOM	4258	CB	GLU	D	96	84.392	85.213	-2.937	1.00	47.59	D
ATOM	4259	CG	GLU	D	96	83.007	84.620	-2.777	1.00	47.59	D
ATOM	4260	CD	GLU	D	96	82.672	83.615	-3.862	1.00	47.59	D
ATOM	4261	OE1	GLU	D	96	83.309	83.676	-4.930	1.00	47.59	D
ATOM	4262	OE2	GLU	D	96	81.777	82.767	-3.660	1.00	47.59	D
ATOM	4263	C	GLU	D	96	85.287	84.351	-0.811	1.00	37.43	D
ATOM	4264	O	GLU	D	96	86.035	83.470	-1.244	1.00	37.43	D
ATOM	4265	N	PHE	D	97	84.678	84.260	0.367	1.00	50.19	D
ATOM	4266	CA	PHE	D	97	84.848	83.083	1.202	1.00	50.19	D
ATOM	4267	CB	PHE	D	97	84.579	83.412	2.654	1.00	33.14	D
ATOM	4268	CG	PHE	D	97	85.804	83.787	3.422	1.00	33.14	D
ATOM	4269	CD1	PHE	D	97	86.515	84.937	3.108	1.00	33.14	D
ATOM	4270	CD2	PHE	D	97	86.243	82.994	4.476	1.00	33.14	D
ATOM	4271	CE1	PHE	D	97	87.653	85.297	3.833	1.00	33.14	D
ATOM	4272	CE2	PHE	D	97	87.383	83.340	5.212	1.00	33.14	D
ATOM	4273	CZ	PHE	D	97	88.088	84.498	4.890	1.00	33.14	D
ATOM	4274	C	PHE	D	97	83.935	81.954	0.771	1.00	50.19	D
ATOM	4275	O	PHE	D	97	82.754	82.158	0.478	1.00	50.19	D
ATOM	4276	N	ILE	D	98	84.499	80.756	0.731	1.00	34.44	D
ATOM	4277	CA	ILE	D	98	83.757	79.574	0.341	1.00	34.44	D
ATOM	4278	CB	ILE	D	98	84.413	78.903	-0.874	1.00	44.32	D
ATOM	4279	CG2	ILE	D	98	83.565	77.727	-1.340	1.00	44.32	D
ATOM	4280	CG1	ILE	D	98	84.580	79.937	-1.991	1.00	44.32	D
ATOM	4281	CD1	ILE	D	98	85.394	79.465	-3.168	1.00	44.32	D
ATOM	4282	C	ILE	D	98	83.742	78.606	1.516	1.00	34.44	D
ATOM	4283	O	ILE	D	98	84.788	78.151	1.983	1.00	34.44	D
ATOM	4284	N	SER	D	99	82.544	78.300	1.996	1.00	40.20	D
ATOM	4285	CA	SER	D	99	82.393	77.400	3.122	1.00	40.20	D
ATOM	4286	CB	SER	D	99	81.057	77.661	3.814	1.00	50.16	D
ATOM	4287	OG	SER	D	99	81.026	77.009	5.070	1.00	50.16	D
ATOM	4288	C	SER	D	99	82.466	75.963	2.635	1.00	40.20	D
ATOM	4289	O	SER	D	99	81.514	75.445	2.060	1.00	40.20	D
ATOM	4290	N	ILE	D	100	83.601	75.319	2.863	1.00	40.10	D
ATOM	4291	CA	ILE	D	100	83.787	73.942	2.431	1.00	40.10	D
ATOM	4292	CB	ILE	D	100	85.296	73.558	2.426	1.00	34.87	D
ATOM	4293	CG2	ILE	D	100	85.471	72.097	1.992	1.00	34.87	D
ATOM	4294	CG1	ILE	D	100	86.071	74.482	1.464	1.00	34.87	D
ATOM	4295	CD1	ILE	D	100	85.612	74.400	0.003	1.00	34.87	D
ATOM	4296	C	ILE	D	100	83.020	73.009	3.356	1.00	40.10	D
ATOM	4297	O	ILE	D	100	82.278	72.145	2.905	1.00	40.10	D
ATOM	4298	N	ALA	D	101	83.197	73.214	4.655	1.00	41.36	D
ATOM	4299	CA	ALA	D	101	82.546	72.427	5.690	1.00	41.36	D

FIGURE 2 Continued

ATOM	4300	CB	ALA	D	101	83.238	71.082	5.826	1.00	24.32	D
ATOM	4301	C	ALA	D	101	82.719	73.248	6.965	1.00	41.36	D
ATOM	4302	O	ALA	D	101	83.469	74.228	6.964	1.00	41.36	D
ATOM	4303	N	VAL	D	102	82.042	72.882	8.051	1.00	37.27	D
ATOM	4304	CA	VAL	D	102	82.219	73.664	9.269	1.00	37.27	D
ATOM	4305	CB	VAL	D	102	81.302	73.180	10.454	1.00	43.49	D
ATOM	4306	CG1	VAL	D	102	79.879	72.964	9.956	1.00	43.49	D
ATOM	4307	CG2	VAL	D	102	81.841	71.919	11.082	1.00	43.49	D
ATOM	4308	C	VAL	D	102	83.688	73.552	9.650	1.00	37.27	D
ATOM	4309	O	VAL	D	102	84.252	72.454	9.717	1.00	37.27	D
ATOM	4310	N	GLY	D	103	84.315	74.700	9.852	1.00	36.63	D
ATOM	4311	CA	GLY	D	103	85.717	74.726	10.210	1.00	36.63	D
ATOM	4312	C	GLY	D	103	86.636	74.795	9.010	1.00	36.63	D
ATOM	4313	O	GLY	D	103	87.833	75.019	9.168	1.00	36.63	D
ATOM	4314	N	LEU	D	104	86.093	74.621	7.810	1.00	31.40	D
ATOM	4315	CA	LEU	D	104	86.922	74.639	6.612	1.00	31.40	D
ATOM	4316	CB	LEU	D	104	86.944	73.255	5.963	1.00	33.42	D
ATOM	4317	CG	LEU	D	104	87.448	72.103	6.822	1.00	33.42	D
ATOM	4318	CD1	LEU	D	104	87.385	70.810	6.018	1.00	33.42	D
ATOM	4319	CD2	LEU	D	104	88.870	72.403	7.280	1.00	33.42	D
ATOM	4320	C	LEU	D	104	86.491	75.646	5.567	1.00	31.40	D
ATOM	4321	O	LEU	D	104	85.316	75.707	5.194	1.00	31.40	D
ATOM	4322	N	VAL	D	105	87.447	76.419	5.063	1.00	32.85	D
ATOM	4323	CA	VAL	D	105	87.115	77.408	4.051	1.00	32.85	D
ATOM	4324	CB	VAL	D	105	87.151	78.854	4.623	1.00	28.26	D
ATOM	4325	CG1	VAL	D	105	86.236	78.972	5.823	1.00	28.26	D
ATOM	4326	CG2	VAL	D	105	88.588	79.214	5.005	1.00	28.26	D
ATOM	4327	C	VAL	D	105	88.075	77.391	2.875	1.00	32.85	D
ATOM	4328	O	VAL	D	105	89.135	76.761	2.908	1.00	32.85	D
ATOM	4329	N	SER	D	106	87.659	78.092	1.833	1.00	35.69	D
ATOM	4330	CA	SER	D	106	88.453	78.300	0.644	1.00	35.69	D
ATOM	4331	CB	SER	D	106	87.910	77.514	-0.549	1.00	34.35	D
ATOM	4332	OG	SER	D	106	88.341	76.166	-0.476	1.00	34.35	D
ATOM	4333	C	SER	D	106	88.281	79.801	0.440	1.00	35.69	D
ATOM	4334	O	SER	D	106	87.247	80.368	0.799	1.00	35.69	D
ATOM	4335	N	ILE	D	107	89.298	80.445	-0.109	1.00	38.83	D
ATOM	4336	CA	ILE	D	107	89.255	81.876	-0.321	1.00	38.83	D
ATOM	4337	CB	ILE	D	107	90.227	82.575	0.644	1.00	32.55	D
ATOM	4338	CG2	ILE	D	107	90.178	84.078	0.434	1.00	32.55	D
ATOM	4339	CG1	ILE	D	107	89.869	82.200	2.087	1.00	32.55	D
ATOM	4340	CD1	ILE	D	107	90.972	82.435	3.072	1.00	32.55	D
ATOM	4341	C	ILE	D	107	89.641	82.205	-1.750	1.00	38.83	D
ATOM	4342	O	ILE	D	107	90.769	81.951	-2.167	1.00	38.83	D
ATOM	4343	N	ARG	D	108	88.699	82.761	-2.503	1.00	34.65	D
ATOM	4344	CA	ARG	D	108	88.964	83.125	-3.882	1.00	34.65	D
ATOM	4345	CB	ARG	D	108	87.893	82.552	-4.808	1.00	56.81	D
ATOM	4346	CG	ARG	D	108	88.035	83.065	-6.222	1.00	56.81	D
ATOM	4347	CD	ARG	D	108	87.762	82.009	-7.256	1.00	56.81	D
ATOM	4348	NE	ARG	D	108	86.366	81.976	-7.662	1.00	56.81	D
ATOM	4349	CZ	ARG	D	108	85.963	81.744	-8.909	1.00	56.81	D
ATOM	4350	NH1	ARG	D	108	86.856	81.529	-9.870	1.00	56.81	D
ATOM	4351	NH2	ARG	D	108	84.667	81.728	-9.197	1.00	56.81	D
ATOM	4352	C	ARG	D	108	89.041	84.636	-4.090	1.00	34.65	D
ATOM	4353	O	ARG	D	108	88.171	85.386	-3.631	1.00	34.65	D
ATOM	4354	N	GLY	D	109	90.088	85.081	-4.786	1.00	42.88	D
ATOM	4355	CA	GLY	D	109	90.225	86.499	-5.062	1.00	42.88	D
ATOM	4356	C	GLY	D	109	89.118	86.866	-6.033	1.00	42.88	D

FIGURE 2 Continued

ATOM	4357	O	GLY	D	109	88.973	86.238	-7.082	1.00	42.88	D
ATOM	4358	N	VAL	D	110	88.319	87.868	-5.692	1.00	48.85	D
ATOM	4359	CA	VAL	D	110	87.232	88.263	-6.567	1.00	48.85	D
ATOM	4360	CB	VAL	D	110	86.339	89.308	-5.891	1.00	40.18	D
ATOM	4361	CG1	VAL	D	110	85.258	89.771	-6.852	1.00	40.18	D
ATOM	4362	CG2	VAL	D	110	85.719	88.707	-4.640	1.00	40.18	D
ATOM	4363	C	VAL	D	110	87.719	88.806	-7.906	1.00	48.85	D
ATOM	4364	O	VAL	D	110	87.185	88.454	-8.955	1.00	48.85	D
ATOM	4365	N	ASP	D	111	88.732	89.661	-7.880	1.00	48.31	D
ATOM	4366	CA	ASP	D	111	89.242	90.222	-9.118	1.00	48.31	D
ATOM	4367	CB	ASP	D	111	90.166	91.403	-8.826	1.00	76.83	D
ATOM	4368	CG	ASP	D	111	90.454	92.234	-10.061	1.00	76.83	D
ATOM	4369	OD1	ASP	D	111	90.994	91.678	-11.036	1.00	76.83	D
ATOM	4370	OD2	ASP	D	111	90.139	93.441	-10.060	1.00	76.83	D
ATOM	4371	C	ASP	D	111	89.996	89.158	-9.908	1.00	48.31	D
ATOM	4372	O	ASP	D	111	89.596	88.798	-11.009	1.00	48.31	D
ATOM	4373	N	SER	D	112	91.079	88.646	-9.334	1.00	51.84	D
ATOM	4374	CA	SER	D	112	91.897	87.631	-9.990	1.00	51.84	D
ATOM	4375	CB	SER	D	112	93.093	87.279	-9.124	1.00	44.88	D
ATOM	4376	OG	SER	D	112	92.671	86.465	-8.050	1.00	44.88	D
ATOM	4377	C	SER	D	112	91.153	86.347	-10.293	1.00	51.84	D
ATOM	4378	O	SER	D	112	91.441	85.689	-11.282	1.00	51.84	D
ATOM	4379	N	GLY	D	113	90.212	85.977	-9.434	1.00	39.75	D
ATOM	4380	CA	GLY	D	113	89.465	84.750	-9.648	1.00	39.75	D
ATOM	4381	C	GLY	D	113	90.252	83.541	-9.163	1.00	39.75	D
ATOM	4382	O	GLY	D	113	89.817	82.403	-9.324	1.00	39.75	D
ATOM	4383	N	LEU	D	114	91.409	83.779	-8.555	1.00	43.32	D
ATOM	4384	CA	LEU	D	114	92.243	82.683	-8.079	1.00	43.32	D
ATOM	4385	CB	LEU	D	114	93.732	83.028	-8.265	1.00	37.81	D
ATOM	4386	CG	LEU	D	114	94.210	83.444	-9.666	1.00	37.81	D
ATOM	4387	CD1	LEU	D	114	95.642	83.932	-9.567	1.00	37.81	D
ATOM	4388	CD2	LEU	D	114	94.089	82.290	-10.651	1.00	37.81	D
ATOM	4389	C	LEU	D	114	91.993	82.319	-6.618	1.00	43.32	D
ATOM	4390	O	LEU	D	114	91.622	83.166	-5.800	1.00	43.32	D
ATOM	4391	N	TYR	D	115	92.216	81.052	-6.294	1.00	38.40	D
ATOM	4392	CA	TYR	D	115	92.033	80.572	-4.937	1.00	38.40	D
ATOM	4393	CB	TYR	D	115	91.502	79.139	-4.939	1.00	44.55	D
ATOM	4394	CG	TYR	D	115	90.193	78.971	-5.669	1.00	44.55	D
ATOM	4395	CD1	TYR	D	115	90.157	78.815	-7.049	1.00	44.55	D
ATOM	4396	CE1	TYR	D	115	88.949	78.657	-7.717	1.00	44.55	D
ATOM	4397	CD2	TYR	D	115	88.987	78.969	-4.975	1.00	44.55	D
ATOM	4398	CE2	TYR	D	115	87.774	78.812	-5.630	1.00	44.55	D
ATOM	4399	CZ	TYR	D	115	87.759	78.655	-6.997	1.00	44.55	D
ATOM	4400	OH	TYR	D	115	86.555	78.487	-7.644	1.00	44.55	D
ATOM	4401	C	TYR	D	115	93.339	80.615	-4.156	1.00	38.40	D
ATOM	4402	O	TYR	D	115	94.415	80.400	-4.701	1.00	38.40	D
ATOM	4403	N	LEU	D	116	93.231	80.915	-2.873	1.00	33.54	D
ATOM	4404	CA	LEU	D	116	94.385	80.955	-2.013	1.00	33.54	D
ATOM	4405	CB	LEU	D	116	94.019	81.604	-0.682	1.00	29.09	D
ATOM	4406	CG	LEU	D	116	95.118	81.572	0.375	1.00	29.09	D
ATOM	4407	CD1	LEU	D	116	96.258	82.500	-0.040	1.00	29.09	D
ATOM	4408	CD2	LEU	D	116	94.549	81.999	1.717	1.00	29.09	D
ATOM	4409	C	LEU	D	116	94.787	79.508	-1.778	1.00	33.54	D
ATOM	4410	O	LEU	D	116	93.942	78.654	-1.496	1.00	33.54	D
ATOM	4411	N	GLY	D	117	96.077	79.226	-1.898	1.00	37.70	D
ATOM	4412	CA	GLY	D	117	96.546	77.875	-1.675	1.00	37.70	D
ATOM	4413	C	GLY	D	117	97.846	77.913	-0.915	1.00	37.70	D

FIGURE 2 Continued

ATOM	4414	O	GLY	D	117	98.467	78.967	-0.780	1.00	37.70	D
ATOM	4415	N	MET	D	118	98.244	76.767	-0.387	1.00	42.09	D
ATOM	4416	CA	MET	D	118	99.503	76.660	0.327	1.00	42.09	D
ATOM	4417	CB	MET	D	118	99.277	76.692	1.832	1.00	42.40	D
ATOM	4418	CG	MET	D	118	100.561	76.793	2.604	1.00	42.40	D
ATOM	4419	SD	MET	D	118	100.350	76.460	4.354	1.00	42.40	D
ATOM	4420	CE	MET	D	118	99.969	78.117	4.973	1.00	42.40	D
ATOM	4421	C	MET	D	118	100.127	75.328	-0.086	1.00	42.09	D
ATOM	4422	O	MET	D	118	99.503	74.272	0.056	1.00	42.09	D
ATOM	4423	N	ASN	D	119	101.347	75.376	-0.618	1.00	53.96	D
ATOM	4424	CA	ASN	D	119	102.014	74.153	-1.051	1.00	53.96	D
ATOM	4425	CB	ASN	D	119	103.024	74.442	-2.163	1.00	41.18	D
ATOM	4426	CG	ASN	D	119	104.117	75.402	-1.737	1.00	41.18	D
ATOM	4427	OD1	ASN	D	119	104.489	75.470	-0.560	1.00	41.18	D
ATOM	4428	ND2	ASN	D	119	104.655	76.141	-2.702	1.00	41.18	D
ATOM	4429	C	ASN	D	119	102.704	73.455	0.106	1.00	53.96	D
ATOM	4430	O	ASN	D	119	102.711	73.963	1.226	1.00	53.96	D
ATOM	4431	N	GLU	D	120	103.286	72.292	-0.178	1.00	63.37	D
ATOM	4432	CA	GLU	D	120	103.965	71.488	0.835	1.00	63.37	D
ATOM	4433	CB	GLU	D	120	104.493	70.192	0.214	1.00	82.96	D
ATOM	4434	CG	GLU	D	120	104.737	69.097	1.240	1.00	82.96	D
ATOM	4435	CD	GLU	D	120	104.925	67.722	0.621	1.00	82.96	D
ATOM	4436	OE1	GLU	D	120	104.210	67.395	-0.354	1.00	82.96	D
ATOM	4437	OE2	GLU	D	120	105.775	66.959	1.128	1.00	82.96	D
ATOM	4438	C	GLU	D	120	105.094	72.230	1.541	1.00	63.37	D
ATOM	4439	O	GLU	D	120	105.503	71.844	2.638	1.00	63.37	D
ATOM	4440	N	LYS	D	121	105.602	73.289	0.915	1.00	52.24	D
ATOM	4441	CA	LYS	D	121	106.664	74.080	1.523	1.00	52.24	D
ATOM	4442	CB	LYS	D	121	107.547	74.744	0.466	1.00	65.90	D
ATOM	4443	CG	LYS	D	121	108.528	73.821	-0.230	1.00	65.90	D
ATOM	4444	CD	LYS	D	121	109.721	74.625	-0.735	1.00	65.90	D
ATOM	4445	CE	LYS	D	121	110.632	73.813	-1.651	1.00	65.90	D
ATOM	4446	NZ	LYS	D	121	109.999	73.498	-2.977	1.00	65.90	D
ATOM	4447	C	LYS	D	121	106.029	75.161	2.378	1.00	52.24	D
ATOM	4448	O	LYS	D	121	106.727	75.984	2.981	1.00	52.24	D
ATOM	4449	N	GLY	D	122	104.698	75.161	2.415	1.00	42.67	D
ATOM	4450	CA	GLY	D	122	103.974	76.145	3.197	1.00	42.67	D
ATOM	4451	C	GLY	D	122	103.935	77.517	2.558	1.00	42.67	D
ATOM	4452	O	GLY	D	122	103.812	78.514	3.252	1.00	42.67	D
ATOM	4453	N	GLU	D	123	104.024	77.572	1.233	1.00	47.74	D
ATOM	4454	CA	GLU	D	123	104.003	78.851	0.521	1.00	47.74	D
ATOM	4455	CB	GLU	D	123	105.048	78.858	-0.609	1.00	70.94	D
ATOM	4456	CG	GLU	D	123	106.492	78.709	-0.135	1.00	70.94	D
ATOM	4457	CD	GLU	D	123	107.503	78.706	-1.280	1.00	70.94	D
ATOM	4458	OE1	GLU	D	123	107.343	77.896	-2.227	1.00	70.94	D
ATOM	4459	OE2	GLU	D	123	108.460	79.511	-1.222	1.00	70.94	D
ATOM	4460	C	GLU	D	123	102.626	79.161	-0.051	1.00	47.74	D
ATOM	4461	O	GLU	D	123	101.985	78.310	-0.674	1.00	47.74	D
ATOM	4462	N	LEU	D	124	102.188	80.395	0.164	1.00	42.34	D
ATOM	4463	CA	LEU	D	124	100.886	80.847	-0.309	1.00	42.34	D
ATOM	4464	CB	LEU	D	124	100.442	82.088	0.471	1.00	32.52	D
ATOM	4465	CG	LEU	D	124	100.357	81.867	1.986	1.00	32.52	D
ATOM	4466	CD1	LEU	D	124	100.065	83.181	2.704	1.00	32.52	D
ATOM	4467	CD2	LEU	D	124	99.291	80.831	2.263	1.00	32.52	D
ATOM	4468	C	LEU	D	124	100.958	81.176	-1.780	1.00	42.34	D
ATOM	4469	O	LEU	D	124	102.020	81.518	-2.287	1.00	42.34	D
ATOM	4470	N	TYR	D	125	99.831	81.080	-2.468	1.00	44.44	D

FIGURE 2 Continued

ATOM	4471	CA	TYR	D	125	99.820	81.392	-3.882	1.00	44.44	D
ATOM	4472	CB	TYR	D	125	100.692	80.382	-4.641	1.00	31.44	D
ATOM	4473	CG	TYR	D	125	100.120	78.977	-4.693	1.00	31.44	D
ATOM	4474	CD1	TYR	D	125	99.250	78.604	-5.711	1.00	31.44	D
ATOM	4475	CE1	TYR	D	125	98.683	77.338	-5.744	1.00	31.44	D
ATOM	4476	CD2	TYR	D	125	100.415	78.037	-3.694	1.00	31.44	D
ATOM	4477	CE2	TYR	D	125	99.842	76.760	-3.716	1.00	31.44	D
ATOM	4478	CZ	TYR	D	125	98.978	76.423	-4.748	1.00	31.44	D
ATOM	4479	OH	TYR	D	125	98.383	75.178	-4.802	1.00	31.44	D
ATOM	4480	C	TYR	D	125	98.392	81.352	-4.397	1.00	44.44	D
ATOM	4481	O	TYR	D	125	97.518	80.760	-3.761	1.00	44.44	D
ATOM	4482	N	GLY	D	126	98.163	81.991	-5.540	1.00	40.42	D
ATOM	4483	CA	GLY	D	126	96.843	82.000	-6.134	1.00	40.42	D
ATOM	4484	C	GLY	D	126	96.752	80.814	-7.064	1.00	40.42	D
ATOM	4485	O	GLY	D	126	97.617	80.632	-7.914	1.00	40.42	D
ATOM	4486	N	SER	D	127	95.713	80.002	-6.912	1.00	42.64	D
ATOM	4487	CA	SER	D	127	95.547	78.819	-7.743	1.00	42.64	D
ATOM	4488	CB	SER	D	127	95.313	77.602	-6.841	1.00	40.20	D
ATOM	4489	OG	SER	D	127	95.106	76.413	-7.587	1.00	40.20	D
ATOM	4490	C	SER	D	127	94.399	78.969	-8.746	1.00	42.64	D
ATOM	4491	O	SER	D	127	93.323	79.449	-8.403	1.00	42.64	D
ATOM	4492	N	GLU	D	128	94.632	78.565	-9.989	1.00	50.37	D
ATOM	4493	CA	GLU	D	128	93.598	78.647	-11.015	1.00	50.37	D
ATOM	4494	CB	GLU	D	128	94.175	78.257	-12.377	1.00	100.00	D
ATOM	4495	CG	GLU	D	128	93.173	78.296	-13.522	1.00	100.00	D
ATOM	4496	CD	GLU	D	128	93.692	77.604	-14.777	1.00	100.00	D
ATOM	4497	OE1	GLU	D	128	93.858	76.363	-14.754	1.00	100.00	D
ATOM	4498	OE2	GLU	D	128	93.937	78.301	-15.785	1.00	100.00	D
ATOM	4499	C	GLU	D	128	92.463	77.691	-10.649	1.00	50.37	D
ATOM	4500	O	GLU	D	128	91.285	78.004	-10.813	1.00	50.37	D
ATOM	4501	N	LYS	D	129	92.833	76.521	-10.143	1.00	52.50	D
ATOM	4502	CA	LYS	D	129	91.856	75.514	-9.764	1.00	52.50	D
ATOM	4503	CB	LYS	D	129	92.219	74.166	-10.389	1.00	86.48	D
ATOM	4504	CG	LYS	D	129	92.266	74.186	-11.903	1.00	86.48	D
ATOM	4505	CD	LYS	D	129	92.522	72.804	-12.470	1.00	86.48	D
ATOM	4506	CE	LYS	D	129	92.682	72.859	-13.980	1.00	86.48	D
ATOM	4507	NZ	LYS	D	129	91.497	73.480	-14.631	1.00	86.48	D
ATOM	4508	C	LYS	D	129	91.747	75.356	-8.258	1.00	52.50	D
ATOM	4509	O	LYS	D	129	92.703	75.592	-7.520	1.00	52.50	D
ATOM	4510	N	LEU	D	130	90.561	74.967	-7.811	1.00	37.77	D
ATOM	4511	CA	LEU	D	130	90.311	74.745	-6.402	1.00	37.77	D
ATOM	4512	CB	LEU	D	130	88.810	74.832	-6.126	1.00	43.69	D
ATOM	4513	CG	LEU	D	130	88.319	74.566	-4.700	1.00	43.69	D
ATOM	4514	CD1	LEU	D	130	89.028	75.484	-3.726	1.00	43.69	D
ATOM	4515	CD2	LEU	D	130	86.805	74.774	-4.643	1.00	43.69	D
ATOM	4516	C	LEU	D	130	90.835	73.350	-6.048	1.00	37.77	D
ATOM	4517	O	LEU	D	130	90.176	72.352	-6.313	1.00	37.77	D
ATOM	4518	N	THR	D	131	92.021	73.281	-5.456	1.00	44.53	D
ATOM	4519	CA	THR	D	131	92.595	71.990	-5.091	1.00	44.53	D
ATOM	4520	CB	THR	D	131	94.065	71.866	-5.572	1.00	45.27	D
ATOM	4521	OG1	THR	D	131	94.933	72.596	-4.688	1.00	45.27	D
ATOM	4522	CG2	THR	D	131	94.204	72.424	-6.980	1.00	45.27	D
ATOM	4523	C	THR	D	131	92.560	71.811	-3.580	1.00	44.53	D
ATOM	4524	O	THR	D	131	92.086	72.683	-2.852	1.00	44.53	D
ATOM	4525	N	GLN	D	132	93.070	70.682	-3.108	1.00	49.31	D
ATOM	4526	CA	GLN	D	132	93.079	70.414	-1.681	1.00	49.31	D
ATOM	4527	CB	GLN	D	132	93.493	68.971	-1.416	1.00	49.07	D

FIGURE 2 Continued

ATOM	4528	CG	GLN	D	132	92.605	67.957	-2.092	1.00	49.07	D
ATOM	4529	CD	GLN	D	132	92.862	66.551	-1.591	1.00	49.07	D
ATOM	4530	OE1	GLN	D	132	92.377	65.575	-2.165	1.00	49.07	D
ATOM	4531	NE2	GLN	D	132	93.624	66.440	-0.506	1.00	49.07	D
ATOM	4532	C	GLN	D	132	94.026	71.369	-0.976	1.00	49.31	D
ATOM	4533	O	GLN	D	132	93.977	71.530	0.244	1.00	49.31	D
ATOM	4534	N	GLU	D	133	94.892	72.010	-1.748	1.00	39.41	D
ATOM	4535	CA	GLU	D	133	95.828	72.950	-1.156	1.00	39.41	D
ATOM	4536	CB	GLU	D	133	97.005	73.196	-2.093	1.00	50.87	D
ATOM	4537	CG	GLU	D	133	97.725	71.948	-2.514	1.00	50.87	D
ATOM	4538	CD	GLU	D	133	99.155	72.232	-2.870	1.00	50.87	D
ATOM	4539	OE1	GLU	D	133	99.407	73.240	-3.560	1.00	50.87	D
ATOM	4540	OE2	GLU	D	133	100.030	71.447	-2.458	1.00	50.87	D
ATOM	4541	C	GLU	D	133	95.120	74.264	-0.893	1.00	39.41	D
ATOM	4542	O	GLU	D	133	95.673	75.160	-0.262	1.00	39.41	D
ATOM	4543	N	CYS	D	134	93.889	74.366	-1.376	1.00	42.39	D
ATOM	4544	CA	CYS	D	134	93.111	75.585	-1.222	1.00	42.39	D
ATOM	4545	CB	CYS	D	134	92.427	75.914	-2.545	1.00	45.18	D
ATOM	4546	SG	CYS	D	134	93.588	75.980	-3.909	1.00	45.18	D
ATOM	4547	C	CYS	D	134	92.071	75.509	-0.113	1.00	42.39	D
ATOM	4548	O	CYS	D	134	91.186	76.352	-0.027	1.00	42.39	D
ATOM	4549	N	VAL	D	135	92.186	74.505	0.741	1.00	38.89	D
ATOM	4550	CA	VAL	D	135	91.239	74.334	1.821	1.00	38.89	D
ATOM	4551	CB	VAL	D	135	90.637	72.926	1.781	1.00	29.51	D
ATOM	4552	CG1	VAL	D	135	89.651	72.749	2.915	1.00	29.51	D
ATOM	4553	CG2	VAL	D	135	89.960	72.703	0.441	1.00	29.51	D
ATOM	4554	C	VAL	D	135	91.922	74.573	3.156	1.00	38.89	D
ATOM	4555	O	VAL	D	135	92.879	73.877	3.514	1.00	38.89	D
ATOM	4556	N	PHE	D	136	91.427	75.558	3.899	1.00	32.74	D
ATOM	4557	CA	PHE	D	136	92.036	75.873	5.174	1.00	32.74	D
ATOM	4558	CB	PHE	D	136	92.561	77.312	5.158	1.00	37.72	D
ATOM	4559	CG	PHE	D	136	93.515	77.600	4.044	1.00	37.72	D
ATOM	4560	CD1	PHE	D	136	93.051	77.807	2.751	1.00	37.72	D
ATOM	4561	CD2	PHE	D	136	94.880	77.675	4.285	1.00	37.72	D
ATOM	4562	CE1	PHE	D	136	93.933	78.089	1.713	1.00	37.72	D
ATOM	4563	CE2	PHE	D	136	95.777	77.959	3.247	1.00	37.72	D
ATOM	4564	CZ	PHE	D	136	95.303	78.165	1.966	1.00	37.72	D
ATOM	4565	C	PHE	D	136	91.145	75.688	6.402	1.00	32.74	D
ATOM	4566	O	PHE	D	136	89.909	75.745	6.333	1.00	32.74	D
ATOM	4567	N	ARG	D	137	91.802	75.466	7.533	1.00	35.24	D
ATOM	4568	CA	ARG	D	137	91.120	75.313	8.799	1.00	35.24	D
ATOM	4569	CB	ARG	D	137	91.952	74.467	9.743	1.00	36.01	D
ATOM	4570	CG	ARG	D	137	92.142	73.053	9.297	1.00	36.01	D
ATOM	4571	CD	ARG	D	137	92.856	72.262	10.380	1.00	36.01	D
ATOM	4572	NE	ARG	D	137	92.976	70.852	10.024	1.00	36.01	D
ATOM	4573	CZ	ARG	D	137	93.439	69.917	10.842	1.00	36.01	D
ATOM	4574	NH1	ARG	D	137	93.829	70.247	12.067	1.00	36.01	D
ATOM	4575	NH2	ARG	D	137	93.500	68.658	10.438	1.00	36.01	D
ATOM	4576	C	ARG	D	137	90.975	76.710	9.382	1.00	35.24	D
ATOM	4577	O	ARG	D	137	91.974	77.364	9.713	1.00	35.24	D
ATOM	4578	N	GLU	D	138	89.730	77.172	9.479	1.00	34.60	D
ATOM	4579	CA	GLU	D	138	89.428	78.486	10.031	1.00	34.60	D
ATOM	4580	CB	GLU	D	138	88.292	79.141	9.238	1.00	37.71	D
ATOM	4581	CG	GLU	D	138	87.700	80.394	9.876	1.00	37.71	D
ATOM	4582	CD	GLU	D	138	86.586	80.978	9.038	1.00	37.71	D
ATOM	4583	OE1	GLU	D	138	86.828	81.907	8.232	1.00	37.71	D
ATOM	4584	OE2	GLU	D	138	85.449	80.488	9.172	1.00	37.71	D

FIGURE 2 Continued

ATOM	4585	C	GLU	D	138	89.009	78.269	11.478	1.00	34.60	D
ATOM	4586	O	GLU	D	138	88.023	77.593	11.756	1.00	34.60	D
ATOM	4587	N	GLN	D	139	89.764	78.837	12.402	1.00	42.07	D
ATOM	4588	CA	GLN	D	139	89.458	78.669	13.810	1.00	42.07	D
ATOM	4589	CB	GLN	D	139	90.325	77.558	14.404	1.00	27.07	D
ATOM	4590	CG	GLN	D	139	90.109	76.224	13.736	1.00	27.07	D
ATOM	4591	CD	GLN	D	139	91.081	75.172	14.201	1.00	27.07	D
ATOM	4592	OE1	GLN	D	139	91.843	75.380	15.152	1.00	27.07	D
ATOM	4593	NE2	GLN	D	139	91.060	74.023	13.535	1.00	27.07	D
ATOM	4594	C	GLN	D	139	89.662	79.954	14.579	1.00	42.07	D
ATOM	4595	O	GLN	D	139	90.679	80.633	14.435	1.00	42.07	D
ATOM	4596	N	PHE	D	140	88.670	80.281	15.393	1.00	32.04	D
ATOM	4597	CA	PHE	D	140	88.694	81.481	16.210	1.00	32.04	D
ATOM	4598	CB	PHE	D	140	87.542	81.430	17.211	1.00	27.68	D
ATOM	4599	CG	PHE	D	140	87.417	82.656	18.041	1.00	27.68	D
ATOM	4600	CD1	PHE	D	140	86.624	83.721	17.612	1.00	27.68	D
ATOM	4601	CD2	PHE	D	140	88.107	82.768	19.247	1.00	27.68	D
ATOM	4602	CE1	PHE	D	140	86.515	84.880	18.376	1.00	27.68	D
ATOM	4603	CE2	PHE	D	140	88.008	83.925	20.021	1.00	27.68	D
ATOM	4604	CZ	PHE	D	140	87.213	84.983	19.587	1.00	27.68	D
ATOM	4605	C	PHE	D	140	90.007	81.596	16.980	1.00	32.04	D
ATOM	4606	O	PHE	D	140	90.534	80.598	17.461	1.00	32.04	D
ATOM	4607	N	GLU	D	141	90.530	82.809	17.097	1.00	36.24	D
ATOM	4608	CA	GLU	D	141	91.755	83.020	17.854	1.00	36.24	D
ATOM	4609	CB	GLU	D	141	92.888	83.506	16.946	1.00	33.76	D
ATOM	4610	CG	GLU	D	141	94.185	83.848	17.695	1.00	33.76	D
ATOM	4611	CD	GLU	D	141	94.843	82.637	18.365	1.00	33.76	D
ATOM	4612	OE1	GLU	D	141	94.561	81.488	17.962	1.00	33.76	D
ATOM	4613	OE2	GLU	D	141	95.665	82.836	19.283	1.00	33.76	D
ATOM	4614	C	GLU	D	141	91.496	84.054	18.955	1.00	36.24	D
ATOM	4615	O	GLU	D	141	91.553	83.728	20.137	1.00	36.24	D
ATOM	4616	N	GLU	D	142	91.209	85.292	18.552	1.00	38.85	D
ATOM	4617	CA	GLU	D	142	90.935	86.379	19.486	1.00	38.85	D
ATOM	4618	CB	GLU	D	142	92.232	86.851	20.148	1.00	50.41	D
ATOM	4619	CG	GLU	D	142	93.399	87.107	19.191	1.00	50.41	D
ATOM	4620	CD	GLU	D	142	93.472	88.539	18.652	1.00	50.41	D
ATOM	4621	OE1	GLU	D	142	92.822	89.443	19.231	1.00	50.41	D
ATOM	4622	OE2	GLU	D	142	94.206	88.760	17.657	1.00	50.41	D
ATOM	4623	C	GLU	D	142	90.234	87.563	18.817	1.00	38.85	D
ATOM	4624	O	GLU	D	142	90.552	87.935	17.682	1.00	38.85	D
ATOM	4625	N	ASN	D	143	89.263	88.134	19.525	1.00	36.40	D
ATOM	4626	CA	ASN	D	143	88.507	89.283	19.035	1.00	36.40	D
ATOM	4627	CB	ASN	D	143	89.342	90.542	19.219	1.00	41.86	D
ATOM	4628	CG	ASN	D	143	89.700	90.769	20.675	1.00	41.86	D
ATOM	4629	OD1	ASN	D	143	88.819	90.972	21.512	1.00	41.86	D
ATOM	4630	ND2	ASN	D	143	90.988	90.710	20.991	1.00	41.86	D
ATOM	4631	C	ASN	D	143	88.028	89.154	17.597	1.00	36.40	D
ATOM	4632	O	ASN	D	143	88.022	90.118	16.832	1.00	36.40	D
ATOM	4633	N	TRP	D	144	87.611	87.941	17.254	1.00	38.51	D
ATOM	4634	CA	TRP	D	144	87.103	87.621	15.938	1.00	38.51	D
ATOM	4635	CB	TRP	D	144	85.967	88.584	15.570	1.00	36.09	D
ATOM	4636	CG	TRP	D	144	84.848	88.416	16.564	1.00	36.09	D
ATOM	4637	CD2	TRP	D	144	84.101	87.212	16.814	1.00	36.09	D
ATOM	4638	CE2	TRP	D	144	83.298	87.449	17.950	1.00	36.09	D
ATOM	4639	CE3	TRP	D	144	84.040	85.954	16.189	1.00	36.09	D
ATOM	4640	CD1	TRP	D	144	84.466	89.307	17.527	1.00	36.09	D
ATOM	4641	NE1	TRP	D	144	83.544	88.734	18.362	1.00	36.09	D

FIGURE 2 Continued

ATOM	4642	CZ2	TRP	D	144	82.439	86.469	18.486	1.00	36.09	D
ATOM	4643	CZ3	TRP	D	144	83.186	84.974	16.723	1.00	36.09	D
ATOM	4644	CH2	TRP	D	144	82.397	85.244	17.860	1.00	36.09	D
ATOM	4645	C	TRP	D	144	88.172	87.515	14.859	1.00	38.51	D
ATOM	4646	O	TRP	D	144	87.881	87.490	13.658	1.00	38.51	D
ATOM	4647	N	TYR	D	145	89.420	87.444	15.307	1.00	36.09	D
ATOM	4648	CA	TYR	D	145	90.530	87.217	14.395	1.00	36.09	D
ATOM	4649	CB	TYR	D	145	91.858	87.715	14.969	1.00	42.84	D
ATOM	4650	CG	TYR	D	145	92.185	89.152	14.679	1.00	42.84	D
ATOM	4651	CD1	TYR	D	145	91.881	90.156	15.592	1.00	42.84	D
ATOM	4652	CE1	TYR	D	145	92.208	91.475	15.326	1.00	42.84	D
ATOM	4653	CD2	TYR	D	145	92.821	89.506	13.490	1.00	42.84	D
ATOM	4654	CE2	TYR	D	145	93.153	90.821	13.211	1.00	42.84	D
ATOM	4655	CZ	TYR	D	145	92.846	91.801	14.130	1.00	42.84	D
ATOM	4656	OH	TYR	D	145	93.182	93.101	13.852	1.00	42.84	D
ATOM	4657	C	TYR	D	145	90.584	85.689	14.350	1.00	36.09	D
ATOM	4658	O	TYR	D	145	90.388	85.028	15.370	1.00	36.09	D
ATOM	4659	N	ASN	D	146	90.829	85.124	13.181	1.00	41.61	D
ATOM	4660	CA	ASN	D	146	90.916	83.679	13.076	1.00	41.61	D
ATOM	4661	CB	ASN	D	146	89.920	83.142	12.052	1.00	28.69	D
ATOM	4662	CG	ASN	D	146	88.497	83.479	12.383	1.00	28.69	D
ATOM	4663	OD1	ASN	D	146	88.023	83.179	13.474	1.00	28.69	D
ATOM	4664	ND2	ASN	D	146	87.794	84.088	11.434	1.00	28.69	D
ATOM	4665	C	ASN	D	146	92.305	83.325	12.587	1.00	41.61	D
ATOM	4666	O	ASN	D	146	93.051	84.187	12.121	1.00	41.61	D
ATOM	4667	N	THR	D	147	92.656	82.054	12.715	1.00	27.33	D
ATOM	4668	CA	THR	D	147	93.924	81.565	12.197	1.00	27.33	D
ATOM	4669	CB	THR	D	147	94.697	80.688	13.201	1.00	29.47	D
ATOM	4670	OG1	THR	D	147	93.852	79.624	13.662	1.00	29.47	D
ATOM	4671	CG2	THR	D	147	95.196	81.525	14.378	1.00	29.47	D
ATOM	4672	C	THR	D	147	93.459	80.685	11.062	1.00	27.33	D
ATOM	4673	O	THR	D	147	92.388	80.092	11.144	1.00	27.33	D
ATOM	4674	N	TYR	D	148	94.237	80.627	9.992	1.00	36.75	D
ATOM	4675	CA	TYR	D	148	93.901	79.786	8.851	1.00	36.75	D
ATOM	4676	CB	TYR	D	148	93.631	80.655	7.625	1.00	29.56	D
ATOM	4677	CG	TYR	D	148	92.384	81.486	7.772	1.00	29.56	D
ATOM	4678	CD1	TYR	D	148	91.146	81.003	7.336	1.00	29.56	D
ATOM	4679	CE1	TYR	D	148	89.975	81.704	7.570	1.00	29.56	D
ATOM	4680	CD2	TYR	D	148	92.418	82.712	8.443	1.00	29.56	D
ATOM	4681	CE2	TYR	D	148	91.251	83.431	8.689	1.00	29.56	D
ATOM	4682	CZ	TYR	D	148	90.031	82.919	8.255	1.00	29.56	D
ATOM	4683	OH	TYR	D	148	88.873	83.599	8.544	1.00	29.56	D
ATOM	4684	C	TYR	D	148	95.096	78.877	8.619	1.00	36.75	D
ATOM	4685	O	TYR	D	148	96.212	79.354	8.405	1.00	36.75	D
ATOM	4686	N	SER	D	149	94.877	77.569	8.699	1.00	36.92	D
ATOM	4687	CA	SER	D	149	95.967	76.631	8.487	1.00	36.92	D
ATOM	4688	CB	SER	D	149	96.349	75.930	9.792	1.00	29.65	D
ATOM	4689	OG	SER	D	149	95.338	75.033	10.215	1.00	29.65	D
ATOM	4690	C	SER	D	149	95.624	75.589	7.435	1.00	36.92	D
ATOM	4691	O	SER	D	149	94.444	75.277	7.207	1.00	36.92	D
ATOM	4692	N	SER	D	150	96.670	75.065	6.787	1.00	36.62	D
ATOM	4693	CA	SER	D	150	96.524	74.047	5.753	1.00	36.62	D
ATOM	4694	CB	SER	D	150	97.898	73.616	5.215	1.00	33.82	D
ATOM	4695	OG	SER	D	150	97.794	72.495	4.340	1.00	33.82	D
ATOM	4696	C	SER	D	150	95.839	72.837	6.346	1.00	36.62	D
ATOM	4697	O	SER	D	150	96.202	72.381	7.433	1.00	36.62	D
ATOM	4698	N	ASN	D	151	94.846	72.317	5.638	1.00	34.37	D

FIGURE 2 Continued

ATOM	4699	CA	ASN	D	151	94.156	71.132	6.117	1.00	34.37	D
ATOM	4700	CB	ASN	D	151	92.671	71.210	5.760	1.00	31.60	D
ATOM	4701	CG	ASN	D	151	91.849	70.124	6.432	1.00	31.60	D
ATOM	4702	OD1	ASN	D	151	91.924	69.942	7.644	1.00	31.60	D
ATOM	4703	ND2	ASN	D	151	91.049	69.406	5.645	1.00	31.60	D
ATOM	4704	C	ASN	D	151	94.814	69.918	5.451	1.00	34.37	D
ATOM	4705	O	ASN	D	151	94.351	68.794	5.579	1.00	34.37	D
ATOM	4706	N	LEU	D	152	95.924	70.164	4.762	1.00	46.72	D
ATOM	4707	CA	LEU	D	152	96.646	69.124	4.041	1.00	46.72	D
ATOM	4708	CB	LEU	D	152	96.731	69.511	2.569	1.00	49.63	D
ATOM	4709	CG	LEU	D	152	97.437	68.610	1.563	1.00	49.63	D
ATOM	4710	CD1	LEU	D	152	96.736	67.264	1.461	1.00	49.63	D
ATOM	4711	CD2	LEU	D	152	97.418	69.312	0.209	1.00	49.63	D
ATOM	4712	C	LEU	D	152	98.047	68.869	4.571	1.00	46.72	D
ATOM	4713	O	LEU	D	152	98.440	67.723	4.765	1.00	46.72	D
ATOM	4714	N	TYR	D	153	98.796	69.939	4.805	1.00	41.01	D
ATOM	4715	CA	TYR	D	153	100.162	69.827	5.294	1.00	41.01	D
ATOM	4716	CB	TYR	D	153	101.097	70.661	4.422	1.00	48.93	D
ATOM	4717	CG	TYR	D	153	100.974	70.372	2.948	1.00	48.93	D
ATOM	4718	CD1	TYR	D	153	101.126	69.075	2.462	1.00	48.93	D
ATOM	4719	CE1	TYR	D	153	101.034	68.799	1.107	1.00	48.93	D
ATOM	4720	CD2	TYR	D	153	100.723	71.393	2.039	1.00	48.93	D

FIGURE 2 Continued

ATOM	4721	CE2	TYR	D	153	100.628	71.132	0.679	1.00	48.93	D
ATOM	4722	CZ	TYR	D	153	100.786	69.831	0.221	1.00	48.93	D
ATOM	4723	OH	TYR	D	153	100.692	69.563	-1.120	1.00	48.93	D
ATOM	4724	C	TYR	D	153	100.281	70.293	6.731	1.00	41.01	D
ATOM	4725	O	TYR	D	153	99.521	71.147	7.172	1.00	41.01	D
ATOM	4726	N	LYS	D	154	101.257	69.746	7.447	1.00	42.63	D
ATOM	4727	CA	LYS	D	154	101.481	70.091	8.847	1.00	42.63	D
ATOM	4728	CB	LYS	D	154	100.459	69.372	9.723	1.00	57.88	D
ATOM	4729	CG	LYS	D	154	100.563	67.863	9.591	1.00	57.88	D
ATOM	4730	CD	LYS	D	154	99.811	67.136	10.672	1.00	57.88	D
ATOM	4731	CE	LYS	D	154	99.973	65.637	10.508	1.00	57.88	D
ATOM	4732	NZ	LYS	D	154	99.252	64.884	11.569	1.00	57.88	D
ATOM	4733	C	LYS	D	154	102.874	69.639	9.275	1.00	42.63	D
ATOM	4734	O	LYS	D	154	103.590	69.019	8.499	1.00	42.63	D
ATOM	4735	N	HIS	D	155	103.250	69.957	10.509	1.00	50.32	D
ATOM	4736	CA	HIS	D	155	104.532	69.527	11.052	1.00	50.32	D
ATOM	4737	CB	HIS	D	155	104.940	70.389	12.247	1.00	44.66	D
ATOM	4738	CG	HIS	D	155	105.301	71.794	11.879	1.00	44.66	D
ATOM	4739	CD2	HIS	D	155	104.641	72.963	12.061	1.00	44.66	D
ATOM	4740	ND1	HIS	D	155	106.468	72.114	11.219	1.00	44.66	D
ATOM	4741	CE1	HIS	D	155	106.512	73.418	11.011	1.00	44.66	D
ATOM	4742	NE2	HIS	D	155	105.414	73.956	11.512	1.00	44.66	D
ATOM	4743	C	HIS	D	155	104.294	68.098	11.509	1.00	50.32	D
ATOM	4744	O	HIS	D	155	103.606	67.864	12.499	1.00	50.32	D
ATOM	4745	N	VAL	D	156	104.855	67.143	10.778	1.00	43.97	D
ATOM	4746	CA	VAL	D	156	104.680	65.735	11.093	1.00	43.97	D
ATOM	4747	CB	VAL	D	156	105.289	64.870	9.973	1.00	43.29	D
ATOM	4748	CG1	VAL	D	156	105.313	63.419	10.377	1.00	43.29	D
ATOM	4749	CG2	VAL	D	156	104.480	65.053	8.689	1.00	43.29	D
ATOM	4750	C	VAL	D	156	105.254	65.307	12.441	1.00	43.97	D
ATOM	4751	O	VAL	D	156	104.805	64.321	13.030	1.00	43.97	D
ATOM	4752	N	ASP	D	157	106.231	66.044	12.952	1.00	44.60	D
ATOM	4753	CA	ASP	D	157	106.819	65.655	14.223	1.00	44.60	D
ATOM	4754	CB	ASP	D	157	108.302	66.046	14.260	1.00	41.65	D
ATOM	4755	CG	ASP	D	157	108.526	67.524	14.041	1.00	41.65	D
ATOM	4756	OD1	ASP	D	157	107.612	68.192	13.513	1.00	41.65	D
ATOM	4757	OD2	ASP	D	157	109.627	68.013	14.383	1.00	41.65	D
ATOM	4758	C	ASP	D	157	106.096	66.171	15.464	1.00	44.60	D
ATOM	4759	O	ASP	D	157	106.047	65.477	16.485	1.00	44.60	D
ATOM	4760	N	THR	D	158	105.524	67.370	15.390	1.00	49.07	D
ATOM	4761	CA	THR	D	158	104.822	67.920	16.548	1.00	49.07	D
ATOM	4762	CB	THR	D	158	105.238	69.367	16.845	1.00	39.02	D
ATOM	4763	OG1	THR	D	158	104.887	70.201	15.732	1.00	39.02	D
ATOM	4764	CG2	THR	D	158	106.734	69.449	17.114	1.00	39.02	D
ATOM	4765	C	THR	D	158	103.315	67.912	16.389	1.00	49.07	D
ATOM	4766	O	THR	D	158	102.580	68.039	17.369	1.00	49.07	D
ATOM	4767	N	GLY	D	159	102.852	67.746	15.158	1.00	35.78	D
ATOM	4768	CA	GLY	D	159	101.423	67.765	14.922	1.00	35.78	D
ATOM	4769	C	GLY	D	159	100.973	69.202	14.690	1.00	35.78	D
ATOM	4770	O	GLY	D	159	99.835	69.439	14.298	1.00	35.78	D
ATOM	4771	N	ARG	D	160	101.869	70.160	14.929	1.00	42.00	D
ATOM	4772	CA	ARG	D	160	101.569	71.580	14.733	1.00	42.00	D
ATOM	4773	CB	ARG	D	160	102.774	72.438	15.102	1.00	74.75	D
ATOM	4774	CG	ARG	D	160	102.630	73.177	16.416	1.00	74.75	D
ATOM	4775	CD	ARG	D	160	102.680	72.248	17.613	1.00	74.75	D

FIGURE 2 Continued

ATOM	4776	NE	ARG	D	160	102.481	72.982	18.862	1.00	74.75	D
ATOM	4777	CZ	ARG	D	160	103.198	74.042	19.234	1.00	74.75	D
ATOM	4778	NH1	ARG	D	160	104.171	74.504	18.459	1.00	74.75	D
ATOM	4779	NH2	ARG	D	160	102.937	74.650	20.385	1.00	74.75	D
ATOM	4780	C	ARG	D	160	101.148	71.901	13.301	1.00	42.00	D
ATOM	4781	O	ARG	D	160	101.535	71.225	12.345	1.00	42.00	D
ATOM	4782	N	ARG	D	161	100.375	72.966	13.153	1.00	37.30	D
ATOM	4783	CA	ARG	D	161	99.855	73.354	11.849	1.00	37.30	D
ATOM	4784	CB	ARG	D	161	98.435	73.858	12.050	1.00	42.99	D
ATOM	4785	CG	ARG	D	161	97.527	72.746	12.508	1.00	42.99	D
ATOM	4786	CD	ARG	D	161	97.188	71.971	11.284	1.00	42.99	D
ATOM	4787	NE	ARG	D	161	97.062	70.547	11.492	1.00	42.99	D
ATOM	4788	CZ	ARG	D	161	96.793	69.696	10.510	1.00	42.99	D
ATOM	4789	NH1	ARG	D	161	96.628	70.137	9.270	1.00	42.99	D
ATOM	4790	NH2	ARG	D	161	96.692	68.404	10.769	1.00	42.99	D
ATOM	4791	C	ARG	D	161	100.660	74.358	11.047	1.00	37.30	D
ATOM	4792	O	ARG	D	161	101.588	74.976	11.555	1.00	37.30	D
ATOM	4793	N	TYR	D	162	100.302	74.487	9.774	1.00	40.61	D
ATOM	4794	CA	TYR	D	162	100.932	75.436	8.856	1.00	40.61	D
ATOM	4795	CB	TYR	D	162	101.105	74.827	7.464	1.00	51.48	D
ATOM	4796	CG	TYR	D	162	102.277	73.905	7.273	1.00	51.48	D
ATOM	4797	CD1	TYR	D	162	103.022	73.441	8.353	1.00	51.48	D
ATOM	4798	CE1	TYR	D	162	104.081	72.564	8.164	1.00	51.48	D
ATOM	4799	CD2	TYR	D	162	102.620	73.471	5.999	1.00	51.48	D
ATOM	4800	CE2	TYR	D	162	103.670	72.594	5.794	1.00	51.48	D
ATOM	4801	CZ	TYR	D	162	104.398	72.142	6.876	1.00	51.48	D
ATOM	4802	OH	TYR	D	162	105.438	71.272	6.665	1.00	51.48	D
ATOM	4803	C	TYR	D	162	99.946	76.589	8.728	1.00	40.61	D
ATOM	4804	O	TYR	D	162	98.896	76.437	8.087	1.00	40.61	D
ATOM	4805	N	TYR	D	163	100.272	77.739	9.307	1.00	49.07	D
ATOM	4806	CA	TYR	D	163	99.362	78.874	9.249	1.00	49.07	D
ATOM	4807	CB	TYR	D	163	99.312	79.590	10.601	1.00	39.23	D
ATOM	4808	CG	TYR	D	163	98.743	78.731	11.698	1.00	39.23	D
ATOM	4809	CD1	TYR	D	163	99.548	77.825	12.389	1.00	39.23	D
ATOM	4810	CE1	TYR	D	163	99.019	76.986	13.358	1.00	39.23	D
ATOM	4811	CD2	TYR	D	163	97.387	78.777	12.007	1.00	39.23	D
ATOM	4812	CE2	TYR	D	163	96.849	77.942	12.970	1.00	39.23	D
ATOM	4813	CZ	TYR	D	163	97.670	77.047	13.643	1.00	39.23	D
ATOM	4814	OH	TYR	D	163	97.132	76.210	14.585	1.00	39.23	D
ATOM	4815	C	TYR	D	163	99.624	79.908	8.185	1.00	49.07	D
ATOM	4816	O	TYR	D	163	100.768	80.209	7.852	1.00	49.07	D
ATOM	4817	N	VAL	D	164	98.536	80.447	7.647	1.00	34.49	D
ATOM	4818	CA	VAL	D	164	98.625	81.511	6.673	1.00	34.49	D
ATOM	4819	CB	VAL	D	164	97.243	81.855	6.112	1.00	30.21	D
ATOM	4820	CG1	VAL	D	164	97.335	83.106	5.226	1.00	30.21	D
ATOM	4821	CG2	VAL	D	164	96.693	80.667	5.326	1.00	30.21	D
ATOM	4822	C	VAL	D	164	99.152	82.700	7.481	1.00	34.49	D
ATOM	4823	O	VAL	D	164	98.739	82.911	8.628	1.00	34.49	D
ATOM	4824	N	ALA	D	165	100.070	83.470	6.912	1.00	36.68	D
ATOM	4825	CA	ALA	D	165	100.598	84.603	7.650	1.00	36.68	D
ATOM	4826	CB	ALA	D	165	101.591	84.118	8.711	1.00	25.46	D
ATOM	4827	C	ALA	D	165	101.246	85.657	6.773	1.00	36.68	D
ATOM	4828	O	ALA	D	165	101.759	85.354	5.695	1.00	36.68	D
ATOM	4829	N	LEU	D	166	101.193	86.900	7.245	1.00	47.49	D
ATOM	4830	CA	LEU	D	166	101.781	88.038	6.554	1.00	47.49	D

FIGURE 2 Continued

ATOM	4831	CB	LEU	D	166	100.703	89.026	6.115	1.00	42.29	D
ATOM	4832	CG	LEU	D	166	99.750	88.578	5.007	1.00	42.29	D
ATOM	4833	CD1	LEU	D	166	98.717	89.667	4.751	1.00	42.29	D
ATOM	4834	CD2	LEU	D	166	100.534	88.293	3.747	1.00	42.29	D
ATOM	4835	C	LEU	D	166	102.719	88.722	7.533	1.00	47.49	D
ATOM	4836	O	LEU	D	166	102.286	89.162	8.599	1.00	47.49	D
ATOM	4837	N	ASN	D	167	103.998	88.814	7.163	1.00	41.94	D
ATOM	4838	CA	ASN	D	167	105.019	89.428	8.010	1.00	41.94	D
ATOM	4839	CB	ASN	D	167	106.375	89.352	7.313	1.00	42.59	D
ATOM	4840	CG	ASN	D	167	106.905	87.949	7.238	1.00	42.59	D
ATOM	4841	OD1	ASN	D	167	107.080	87.287	8.263	1.00	42.59	D
ATOM	4842	ND2	ASN	D	167	107.165	87.477	6.022	1.00	42.59	D
ATOM	4843	C	ASN	D	167	104.750	90.877	8.410	1.00	41.94	D
ATOM	4844	O	ASN	D	167	103.899	91.555	7.816	1.00	41.94	D
ATOM	4845	N	LYS	D	168	105.493	91.347	9.413	1.00	58.07	D
ATOM	4846	CA	LYS	D	168	105.353	92.717	9.894	1.00	58.07	D
ATOM	4847	CB	LYS	D	168	106.375	93.018	10.991	1.00	82.27	D
ATOM	4848	CG	LYS	D	168	106.063	92.336	12.309	1.00	82.27	D
ATOM	4849	CD	LYS	D	168	106.782	92.994	13.486	1.00	82.27	D
ATOM	4850	CE	LYS	D	168	106.294	92.420	14.822	1.00	82.27	D
ATOM	4851	NZ	LYS	D	168	106.876	93.110	16.017	1.00	82.27	D
ATOM	4852	C	LYS	D	168	105.514	93.713	8.755	1.00	58.07	D
ATOM	4853	O	LYS	D	168	105.024	94.836	8.836	1.00	58.07	D
ATOM	4854	N	ASP	D	169	106.184	93.298	7.686	1.00	46.94	D
ATOM	4855	CA	ASP	D	169	106.387	94.175	6.545	1.00	46.94	D
ATOM	4856	CB	ASP	D	169	107.816	94.036	6.028	1.00	66.59	D
ATOM	4857	CG	ASP	D	169	108.050	92.728	5.323	1.00	66.59	D
ATOM	4858	OD1	ASP	D	169	107.378	91.737	5.673	1.00	66.59	D
ATOM	4859	OD2	ASP	D	169	108.913	92.687	4.424	1.00	66.59	D
ATOM	4860	C	ASP	D	169	105.389	93.899	5.420	1.00	46.94	D
ATOM	4861	O	ASP	D	169	105.536	94.417	4.311	1.00	46.94	D
ATOM	4862	N	GLY	D	170	104.381	93.075	5.704	1.00	46.92	D
ATOM	4863	CA	GLY	D	170	103.355	92.788	4.713	1.00	46.92	D
ATOM	4864	C	GLY	D	170	103.666	91.757	3.644	1.00	46.92	D
ATOM	4865	O	GLY	D	170	102.911	91.595	2.687	1.00	46.92	D
ATOM	4866	N	THR	D	171	104.775	91.052	3.790	1.00	38.32	D
ATOM	4867	CA	THR	D	171	105.124	90.039	2.809	1.00	38.32	D
ATOM	4868	CB	THR	D	171	106.651	89.942	2.637	1.00	38.90	D
ATOM	4869	OG1	THR	D	171	107.246	89.498	3.864	1.00	38.90	D
ATOM	4870	CG2	THR	D	171	107.225	91.297	2.289	1.00	38.90	D
ATOM	4871	C	THR	D	171	104.597	88.695	3.293	1.00	38.32	D
ATOM	4872	O	THR	D	171	104.460	88.471	4.498	1.00	38.32	D
ATOM	4873	N	PRO	D	172	104.266	87.791	2.360	1.00	44.57	D
ATOM	4874	CD	PRO	D	172	104.212	87.944	0.896	1.00	46.31	D
ATOM	4875	CA	PRO	D	172	103.765	86.478	2.767	1.00	44.57	D
ATOM	4876	CB	PRO	D	172	103.349	85.844	1.444	1.00	46.31	D
ATOM	4877	CG	PRO	D	172	104.247	86.516	0.437	1.00	46.31	D
ATOM	4878	C	PRO	D	172	104.867	85.698	3.475	1.00	44.57	D
ATOM	4879	O	PRO	D	172	106.020	85.732	3.057	1.00	44.57	D
ATOM	4880	N	ARG	D	173	104.515	85.017	4.558	1.00	37.48	D
ATOM	4881	CA	ARG	D	173	105.473	84.229	5.323	1.00	37.48	D
ATOM	4882	CB	ARG	D	173	105.254	84.464	6.819	1.00	40.07	D
ATOM	4883	CG	ARG	D	173	106.286	83.838	7.734	1.00	40.07	D
ATOM	4884	CD	ARG	D	173	105.855	83.992	9.185	1.00	40.07	D
ATOM	4885	NE	ARG	D	173	106.850	83.523	10.147	1.00	40.07	D

FIGURE 2 Continued

ATOM	4886	CZ	ARG	D	173	108.006	84.133	10.405	1.00	40.07	D
ATOM	4887	NH1	ARG	D	173	108.336	85.254	9.776	1.00	40.07	D
ATOM	4888	NH2	ARG	D	173	108.837	83.618	11.300	1.00	40.07	D
ATOM	4889	C	ARG	D	173	105.248	82.759	4.974	1.00	37.48	D
ATOM	4890	O	ARG	D	173	104.207	82.407	4.414	1.00	37.48	D
ATOM	4891	N	GLU	D	174	106.222	81.906	5.281	1.00	47.99	D
ATOM	4892	CA	GLU	D	174	106.096	80.479	4.993	1.00	47.99	D
ATOM	4893	CB	GLU	D	174	107.468	79.814	4.956	1.00	95.11	D
ATOM	4894	CG	GLU	D	174	108.460	80.471	4.032	1.00	95.11	D
ATOM	4895	CD	GLU	D	174	109.762	79.708	3.977	1.00	95.11	D
ATOM	4896	OE1	GLU	D	174	109.748	78.552	3.499	1.00	95.11	D
ATOM	4897	OE2	GLU	D	174	110.795	80.257	4.419	1.00	95.11	D
ATOM	4898	C	GLU	D	174	105.258	79.825	6.085	1.00	47.99	D
ATOM	4899	O	GLU	D	174	105.514	80.021	7.275	1.00	47.99	D
ATOM	4900	N	GLY	D	175	104.269	79.038	5.678	1.00	39.14	D
ATOM	4901	CA	GLY	D	175	103.413	78.381	6.645	1.00	39.14	D
ATOM	4902	C	GLY	D	175	104.169	77.474	7.590	1.00	39.14	D
ATOM	4903	O	GLY	D	175	103.674	77.123	8.661	1.00	39.14	D
ATOM	4904	N	THR	D	176	105.377	77.096	7.189	1.00	45.29	D
ATOM	4905	CA	THR	D	176	106.219	76.211	7.982	1.00	45.29	D
ATOM	4906	CB	THR	D	176	107.346	75.605	7.126	1.00	45.75	D
ATOM	4907	OG1	THR	D	176	108.078	76.668	6.498	1.00	45.75	D
ATOM	4908	CG2	THR	D	176	106.777	74.669	6.056	1.00	45.75	D
ATOM	4909	C	THR	D	176	106.869	76.943	9.134	1.00	45.29	D
ATOM	4910	O	THR	D	176	107.334	76.319	10.084	1.00	45.29	D
ATOM	4911	N	ARG	D	177	106.898	78.267	9.050	1.00	42.35	D
ATOM	4912	CA	ARG	D	177	107.526	79.079	10.083	1.00	42.35	D
ATOM	4913	CB	ARG	D	177	108.490	80.089	9.447	1.00	65.75	D
ATOM	4914	CG	ARG	D	177	109.524	79.503	8.490	1.00	65.75	D
ATOM	4915	CD	ARG	D	177	110.680	80.478	8.324	1.00	65.75	D
ATOM	4916	NE	ARG	D	177	111.327	80.693	9.614	1.00	65.75	D
ATOM	4917	CZ	ARG	D	177	111.830	81.852	10.028	1.00	65.75	D
ATOM	4918	NH1	ARG	D	177	111.774	82.927	9.247	1.00	65.75	D
ATOM	4919	NH2	ARG	D	177	112.364	81.940	11.242	1.00	65.75	D
ATOM	4920	C	ARG	D	177	106.491	79.837	10.899	1.00	42.35	D
ATOM	4921	O	ARG	D	177	106.658	81.021	11.186	1.00	42.35	D
ATOM	4922	N	THR	D	178	105.427	79.166	11.303	1.00	41.88	D
ATOM	4923	CA	THR	D	178	104.397	79.872	12.045	1.00	41.88	D
ATOM	4924	CB	THR	D	178	103.262	80.301	11.096	1.00	36.87	D
ATOM	4925	OG1	THR	D	178	102.827	79.163	10.340	1.00	36.87	D
ATOM	4926	CG2	THR	D	178	103.751	81.378	10.133	1.00	36.87	D
ATOM	4927	C	THR	D	178	103.798	79.071	13.174	1.00	41.88	D
ATOM	4928	O	THR	D	178	103.663	77.855	13.084	1.00	41.88	D
ATOM	4929	N	LYS	D	179	103.449	79.766	14.249	1.00	43.77	D
ATOM	4930	CA	LYS	D	179	102.815	79.131	15.396	1.00	43.77	D
ATOM	4931	CB	LYS	D	179	103.669	79.308	16.647	1.00	76.20	D
ATOM	4932	CG	LYS	D	179	104.980	78.555	16.562	1.00	76.20	D
ATOM	4933	CD	LYS	D	179	105.610	78.370	17.926	1.00	76.20	D
ATOM	4934	CE	LYS	D	179	106.804	77.423	17.854	1.00	76.20	D
ATOM	4935	NZ	LYS	D	179	107.291	77.045	19.214	1.00	76.20	D
ATOM	4936	C	LYS	D	179	101.467	79.810	15.544	1.00	43.77	D
ATOM	4937	O	LYS	D	179	101.357	81.014	15.325	1.00	43.77	D
ATOM	4938	N	ARG	D	180	100.447	79.037	15.902	1.00	43.98	D
ATOM	4939	CA	ARG	D	180	99.085	79.555	16.032	1.00	43.98	D
ATOM	4940	CB	ARG	D	180	98.181	78.519	16.714	1.00	36.86	D

FIGURE 2 Continued

ATOM	4941	CG	ARG	D	180	96.711	78.951	16.849	1.00	36.86	D
ATOM	4942	CD	ARG	D	180	95.926	78.037	17.786	1.00	36.86	D
ATOM	4943	NE	ARG	D	180	95.647	76.712	17.226	1.00	36.86	D
ATOM	4944	CZ	ARG	D	180	94.565	76.404	16.511	1.00	36.86	D
ATOM	4945	NH1	ARG	D	180	93.641	77.321	16.259	1.00	36.86	D
ATOM	4946	NH2	ARG	D	180	94.403	75.173	16.044	1.00	36.86	D
ATOM	4947	C	ARG	D	180	98.923	80.897	16.741	1.00	43.98	D
ATOM	4948	O	ARG	D	180	98.293	81.809	16.209	1.00	43.98	D
ATOM	4949	N	HIS	D	181	99.503	81.036	17.927	1.00	48.60	D
ATOM	4950	CA	HIS	D	181	99.344	82.274	18.684	1.00	48.60	D
ATOM	4951	CB	HIS	D	181	99.605	81.997	20.161	1.00	41.41	D
ATOM	4952	CG	HIS	D	181	98.677	80.977	20.738	1.00	41.41	D
ATOM	4953	CD2	HIS	D	181	98.917	79.838	21.432	1.00	41.41	D
ATOM	4954	ND1	HIS	D	181	97.310	81.044	20.570	1.00	41.41	D
ATOM	4955	CE1	HIS	D	181	96.747	79.987	21.131	1.00	41.41	D
ATOM	4956	NE2	HIS	D	181	97.699	79.240	21.661	1.00	41.41	D
ATOM	4957	C	HIS	D	181	100.119	83.508	18.241	1.00	48.60	D
ATOM	4958	O	HIS	D	181	99.938	84.591	18.806	1.00	48.60	D
ATOM	4959	N	GLN	D	182	100.968	83.368	17.230	1.00	45.43	D
ATOM	4960	CA	GLN	D	182	101.729	84.516	16.761	1.00	45.43	D
ATOM	4961	CB	GLN	D	182	102.874	84.063	15.870	1.00	46.51	D
ATOM	4962	CG	GLN	D	182	103.944	83.337	16.652	1.00	46.51	D
ATOM	4963	CD	GLN	D	182	105.070	82.858	15.778	1.00	46.51	D
ATOM	4964	OE1	GLN	D	182	104.901	81.940	14.969	1.00	46.51	D
ATOM	4965	NE2	GLN	D	182	106.232	83.482	15.924	1.00	46.51	D
ATOM	4966	C	GLN	D	182	100.834	85.495	16.028	1.00	45.43	D
ATOM	4967	O	GLN	D	182	99.910	85.108	15.321	1.00	45.43	D
ATOM	4968	N	LYS	D	183	101.112	86.773	16.212	1.00	42.01	D
ATOM	4969	CA	LYS	D	183	100.315	87.809	15.593	1.00	42.01	D
ATOM	4970	CB	LYS	D	183	100.899	89.186	15.916	1.00	72.38	D
ATOM	4971	CG	LYS	D	183	100.941	89.489	17.400	1.00	72.38	D
ATOM	4972	CD	LYS	D	183	99.552	89.415	18.019	1.00	72.38	D
ATOM	4973	CE	LYS	D	183	99.609	89.535	19.536	1.00	72.38	D
ATOM	4974	NZ	LYS	D	183	100.233	90.817	19.986	1.00	72.38	D
ATOM	4975	C	LYS	D	183	100.145	87.671	14.091	1.00	42.01	D
ATOM	4976	O	LYS	D	183	99.028	87.830	13.586	1.00	42.01	D
ATOM	4977	N	PHE	D	184	101.219	87.360	13.364	1.00	38.78	D
ATOM	4978	CA	PHE	D	184	101.062	87.294	11.921	1.00	38.78	D
ATOM	4979	CB	PHE	D	184	102.415	87.240	11.191	1.00	52.35	D
ATOM	4980	CG	PHE	D	184	103.415	86.307	11.791	1.00	52.35	D
ATOM	4981	CD1	PHE	D	184	103.083	84.985	12.077	1.00	52.35	D
ATOM	4982	CD2	PHE	D	184	104.717	86.741	12.021	1.00	52.35	D
ATOM	4983	CE1	PHE	D	184	104.040	84.102	12.584	1.00	52.35	D
ATOM	4984	CE2	PHE	D	184	105.682	85.875	12.525	1.00	52.35	D
ATOM	4985	CZ	PHE	D	184	105.345	84.548	12.808	1.00	52.35	D
ATOM	4986	C	PHE	D	184	100.122	86.233	11.387	1.00	38.78	D
ATOM	4987	O	PHE	D	184	99.836	86.227	10.192	1.00	38.78	D
ATOM	4988	N	THR	D	185	99.614	85.357	12.253	1.00	36.57	D
ATOM	4989	CA	THR	D	185	98.671	84.332	11.797	1.00	36.57	D
ATOM	4990	CB	THR	D	185	98.864	82.975	12.510	1.00	41.53	D
ATOM	4991	OG1	THR	D	185	98.443	83.087	13.872	1.00	41.53	D
ATOM	4992	CG2	THR	D	185	100.313	82.546	12.468	1.00	41.53	D
ATOM	4993	C	THR	D	185	97.235	84.785	12.055	1.00	36.57	D
ATOM	4994	O	THR	D	185	96.283	84.158	11.590	1.00	36.57	D
ATOM	4995	N	HIS	D	186	97.081	85.879	12.794	1.00	36.17	D

FIGURE 2 Continued

ATOM	4996	CA	HIS	D	186	95.751	86.398	13.106	1.00	36.17	D
ATOM	4997	CB	HIS	D	186	95.819	87.268	14.361	1.00	37.74	D
ATOM	4998	CG	HIS	D	186	96.372	86.550	15.553	1.00	37.74	D
ATOM	4999	CD2	HIS	D	186	96.859	85.294	15.686	1.00	37.74	D
ATOM	5000	ND1	HIS	D	186	96.451	87.125	16.803	1.00	37.74	D
ATOM	5001	CE1	HIS	D	186	96.962	86.253	17.654	1.00	37.74	D
ATOM	5002	NE2	HIS	D	186	97.217	85.134	17.003	1.00	37.74	D
ATOM	5003	C	HIS	D	186	95.153	87.186	11.944	1.00	36.17	D
ATOM	5004	O	HIS	D	186	95.734	88.163	11.482	1.00	36.17	D
ATOM	5005	N	PHE	D	187	93.994	86.742	11.463	1.00	34.90	D
ATOM	5006	CA	PHE	D	187	93.338	87.404	10.351	1.00	34.90	D
ATOM	5007	CB	PHE	D	187	93.420	86.559	9.079	1.00	43.72	D
ATOM	5008	CG	PHE	D	187	94.775	86.542	8.447	1.00	43.72	D
ATOM	5009	CD1	PHE	D	187	95.786	85.726	8.952	1.00	43.72	D
ATOM	5010	CD2	PHE	D	187	95.047	87.339	7.337	1.00	43.72	D
ATOM	5011	CE1	PHE	D	187	97.051	85.706	8.360	1.00	43.72	D
ATOM	5012	CE2	PHE	D	187	96.313	87.326	6.736	1.00	43.72	D
ATOM	5013	CZ	PHE	D	187	97.312	86.506	7.250	1.00	43.72	D
ATOM	5014	C	PHE	D	187	91.882	87.702	10.647	1.00	34.90	D
ATOM	5015	O	PHE	D	187	91.104	86.823	11.039	1.00	34.90	D
ATOM	5016	N	LEU	D	188	91.508	88.953	10.423	1.00	38.29	D
ATOM	5017	CA	LEU	D	188	90.154	89.378	10.674	1.00	38.29	D
ATOM	5018	CB	LEU	D	188	90.174	90.723	11.386	1.00	35.67	D
ATOM	5019	CG	LEU	D	188	88.818	91.366	11.628	1.00	35.67	D
ATOM	5020	CD1	LEU	D	188	88.028	90.532	12.617	1.00	35.67	D
ATOM	5021	CD2	LEU	D	188	89.026	92.781	12.146	1.00	35.67	D
ATOM	5022	C	LEU	D	188	89.335	89.487	9.401	1.00	38.29	D
ATOM	5023	O	LEU	D	188	89.689	90.225	8.481	1.00	38.29	D
ATOM	5024	N	PRO	D	189	88.243	88.719	9.314	1.00	40.36	D
ATOM	5025	CD	PRO	D	189	87.906	87.527	10.115	1.00	22.38	D
ATOM	5026	CA	PRO	D	189	87.415	88.805	8.108	1.00	40.36	D
ATOM	5027	CB	PRO	D	189	86.483	87.599	8.225	1.00	22.38	D
ATOM	5028	CG	PRO	D	189	87.261	86.623	9.091	1.00	22.38	D
ATOM	5029	C	PRO	D	189	86.656	90.114	8.250	1.00	40.36	D
ATOM	5030	O	PRO	D	189	85.950	90.306	9.227	1.00	40.36	D
ATOM	5031	N	ARG	D	190	86.824	91.025	7.305	1.00	35.97	D
ATOM	5032	CA	ARG	D	190	86.130	92.300	7.363	1.00	35.97	D
ATOM	5033	CB	ARG	D	190	87.118	93.461	7.251	1.00	32.43	D
ATOM	5034	CG	ARG	D	190	88.136	93.574	8.373	1.00	32.43	D
ATOM	5035	CD	ARG	D	190	89.010	94.800	8.127	1.00	32.43	D
ATOM	5036	NE	ARG	D	190	88.194	96.000	7.989	1.00	32.43	D
ATOM	5037	CZ	ARG	D	190	88.340	96.912	7.033	1.00	32.43	D
ATOM	5038	NH1	ARG	D	190	89.278	96.767	6.110	1.00	32.43	D
ATOM	5039	NH2	ARG	D	190	87.542	97.969	7.000	1.00	32.43	D
ATOM	5040	C	ARG	D	190	85.135	92.384	6.215	1.00	35.97	D
ATOM	5041	O	ARG	D	190	85.321	91.764	5.167	1.00	35.97	D
ATOM	5042	N	PRO	D	191	84.055	93.150	6.405	1.00	48.39	D
ATOM	5043	CD	PRO	D	191	83.650	93.840	7.641	1.00	39.44	D
ATOM	5044	CA	PRO	D	191	83.035	93.308	5.373	1.00	48.39	D
ATOM	5045	CB	PRO	D	191	81.893	93.973	6.125	1.00	39.44	D
ATOM	5046	CG	PRO	D	191	82.594	94.789	7.137	1.00	39.44	D
ATOM	5047	C	PRO	D	191	83.524	94.168	4.226	1.00	48.39	D
ATOM	5048	O	PRO	D	191	84.457	94.960	4.377	1.00	48.39	D
ATOM	5049	N	VAL	D	192	82.887	93.998	3.075	1.00	40.09	D
ATOM	5050	CA	VAL	D	192	83.214	94.766	1.890	1.00	40.09	D

FIGURE 2 Continued

ATOM	5051	CB	VAL	D	192	83.335	93.853	0.644	1.00	41.60	D
ATOM	5052	CG1	VAL	D	192	83.502	94.705	-0.609	1.00	41.60	D
ATOM	5053	CG2	VAL	D	192	84.513	92.903	0.802	1.00	41.60	D
ATOM	5054	C	VAL	D	192	82.081	95.763	1.676	1.00	40.09	D
ATOM	5055	O	VAL	D	192	80.895	95.397	1.721	1.00	40.09	D
ATOM	5056	N	ASP	D	193	82.454	97.023	1.469	1.00	45.53	D
ATOM	5057	CA	ASP	D	193	81.495	98.104	1.242	1.00	45.53	D
ATOM	5058	CB	ASP	D	193	82.035	99.416	1.824	1.00	46.23	D
ATOM	5059	CG	ASP	D	193	81.049	100.576	1.701	1.00	46.23	D
ATOM	5060	OD1	ASP	D	193	80.063	100.467	0.932	1.00	46.23	D
ATOM	5061	OD2	ASP	D	193	81.272	101.608	2.374	1.00	46.23	D
ATOM	5062	C	ASP	D	193	81.313	98.247	-0.263	1.00	45.53	D
ATOM	5063	O	ASP	D	193	82.216	98.693	-0.966	1.00	45.53	D
ATOM	5064	N	PRO	D	194	80.141	97.874	-0.776	1.00	58.97	D
ATOM	5065	CD	PRO	D	194	78.954	97.375	-0.065	1.00	48.88	D
ATOM	5066	CA	PRO	D	194	79.885	97.975	-2.214	1.00	58.97	D
ATOM	5067	CB	PRO	D	194	78.400	97.632	-2.319	1.00	48.88	D
ATOM	5068	CG	PRO	D	194	78.196	96.694	-1.169	1.00	48.88	D
ATOM	5069	C	PRO	D	194	80.212	99.356	-2.795	1.00	58.97	D
ATOM	5070	O	PRO	D	194	80.672	99.462	-3.935	1.00	58.97	D
ATOM	5071	N	ASP	D	195	79.974	100.405	-2.010	1.00	70.32	D
ATOM	5072	CA	ASP	D	195	80.238	101.773	-2.454	1.00	70.32	D
ATOM	5073	CB	ASP	D	195	79.792	102.786	-1.389	1.00	75.87	D
ATOM	5074	CG	ASP	D	195	78.298	102.756	-1.132	1.00	75.87	D
ATOM	5075	OD1	ASP	D	195	77.534	102.483	-2.083	1.00	75.87	D
ATOM	5076	OD2	ASP	D	195	77.885	103.025	0.017	1.00	75.87	D
ATOM	5077	C	ASP	D	195	81.706	102.043	-2.782	1.00	70.32	D
ATOM	5078	O	ASP	D	195	82.010	102.908	-3.601	1.00	70.32	D
ATOM	5079	N	LYS	D	196	82.613	101.310	-2.145	1.00	63.50	D
ATOM	5080	CA	LYS	D	196	84.036	101.522	-2.366	1.00	63.50	D
ATOM	5081	CB	LYS	D	196	84.800	101.273	-1.070	1.00	64.38	D
ATOM	5082	CG	LYS	D	196	84.383	102.194	0.053	1.00	64.38	D
ATOM	5083	CD	LYS	D	196	85.336	102.107	1.237	1.00	64.38	D
ATOM	5084	CE	LYS	D	196	84.895	103.043	2.354	1.00	64.38	D
ATOM	5085	NZ	LYS	D	196	84.611	104.410	1.811	1.00	64.38	D
ATOM	5086	C	LYS	D	196	84.669	100.715	-3.490	1.00	63.50	D
ATOM	5087	O	LYS	D	196	85.830	100.931	-3.830	1.00	63.50	D
ATOM	5088	N	VAL	D	197	83.920	99.785	-4.063	1.00	54.17	D
ATOM	5089	CA	VAL	D	197	84.439	98.966	-5.153	1.00	54.17	D
ATOM	5090	CB	VAL	D	197	85.082	97.645	-4.635	1.00	42.93	D
ATOM	5091	CG1	VAL	D	197	86.391	97.944	-3.915	1.00	42.93	D
ATOM	5092	CG2	VAL	D	197	84.116	96.916	-3.693	1.00	42.93	D
ATOM	5093	C	VAL	D	197	83.301	98.617	-6.100	1.00	54.17	D
ATOM	5094	O	VAL	D	197	83.026	97.442	-6.339	1.00	54.17	D
ATOM	5095	N	PRO	D	198	82.635	99.641	-6.666	1.00	72.12	D
ATOM	5096	CD	PRO	D	198	82.941	101.067	-6.463	1.00	59.25	D
ATOM	5097	CA	PRO	D	198	81.510	99.491	-7.596	1.00	72.12	D
ATOM	5098	CB	PRO	D	198	81.219	100.927	-8.017	1.00	59.25	D
ATOM	5099	CG	PRO	D	198	81.631	101.716	-6.824	1.00	59.25	D
ATOM	5100	C	PRO	D	198	81.771	98.590	-8.798	1.00	72.12	D
ATOM	5101	O	PRO	D	198	80.848	97.967	-9.319	1.00	72.12	D
ATOM	5102	N	GLU	D	199	83.023	98.523	-9.237	1.00	98.89	D
ATOM	5103	CA	GLU	D	199	83.371	97.694	-10.384	1.00	98.89	D
ATOM	5104	CB	GLU	D	199	84.871	97.780	-10.680	1.00	93.86	D
ATOM	5105	CG	GLU	D	199	85.527	99.095	-10.299	1.00	93.86	D

FIGURE 2 Continued

ATOM	5106	CD	GLU	D	199	85.787	99.206	-8.804	1.00	93.86	D
ATOM	5107	OE1	GLU	D	199	86.493	98.331	-8.257	1.00	93.86	D
ATOM	5108	OE2	GLU	D	199	85.292	100.167	-8.178	1.00	93.86	D
ATOM	5109	C	GLU	D	199	83.003	96.237	-10.121	1.00	98.89	D
ATOM	5110	O	GLU	D	199	82.685	95.488	-11.048	1.00	98.89	D
ATOM	5111	N	LEU	D	200	83.043	95.840	-8.852	1.00	77.26	D
ATOM	5112	CA	LEU	D	200	82.737	94.468	-8.470	1.00	77.26	D
ATOM	5113	CB	LEU	D	200	83.522	94.099	-7.211	1.00	63.45	D
ATOM	5114	CG	LEU	D	200	85.029	94.384	-7.247	1.00	63.45	D
ATOM	5115	CD1	LEU	D	200	85.669	93.865	-5.969	1.00	63.45	D
ATOM	5116	CD2	LEU	D	200	85.669	93.721	-8.460	1.00	63.45	D
ATOM	5117	C	LEU	D	200	81.249	94.207	-8.246	1.00	77.26	D
ATOM	5118	O	LEU	D	200	80.810	93.061	-8.260	1.00	77.26	D
ATOM	5119	N	TYR	D	201	80.471	95.264	-8.044	1.00	79.23	D
ATOM	5120	CA	TYR	D	201	79.041	95.102	-7.815	1.00	79.23	D
ATOM	5121	CB	TYR	D	201	78.626	95.788	-6.505	1.00	53.35	D
ATOM	5122	CG	TYR	D	201	79.158	95.096	-5.265	1.00	53.35	D
ATOM	5123	CD1	TYR	D	201	80.496	95.214	-4.900	1.00	53.35	D
ATOM	5124	CE1	TYR	D	201	81.009	94.521	-3.815	1.00	53.35	D
ATOM	5125	CD2	TYR	D	201	78.340	94.264	-4.500	1.00	53.35	D
ATOM	5126	CE2	TYR	D	201	78.847	93.564	-3.411	1.00	53.35	D
ATOM	5127	CZ	TYR	D	201	80.183	93.697	-3.077	1.00	53.35	D
ATOM	5128	OH	TYR	D	201	80.704	93.008	-2.009	1.00	53.35	D
ATOM	5129	C	TYR	D	201	78.183	95.620	-8.964	1.00	79.23	D
ATOM	5130	O	TYR	D	201	77.087	96.141	-8.746	1.00	79.23	D
ATOM	5131	N	LYS	D	202	78.677	95.468	-10.190	1.00	99.88	D
ATOM	5132	CA	LYS	D	202	77.931	95.921	-11.359	1.00	99.88	D
ATOM	5133	CB	LYS	D	202	78.812	95.869	-12.609	1.00	100.00	D
ATOM	5134	CG	LYS	D	202	80.025	96.788	-12.550	1.00	100.00	D
ATOM	5135	CD	LYS	D	202	80.778	96.818	-13.878	1.00	100.00	D
ATOM	5136	CE	LYS	D	202	82.027	97.691	-13.791	1.00	100.00	D
ATOM	5137	NZ	LYS	D	202	81.715	99.091	-13.377	1.00	100.00	D
ATOM	5138	C	LYS	D	202	76.683	95.067	-11.567	1.00	99.88	D
ATOM	5139	O	LYS	D	202	75.630	95.581	-11.949	1.00	99.88	D
ATOM	5140	N	ASP	D	203	76.803	93.766	-11.307	1.00	100.00	D
ATOM	5141	CA	ASP	D	203	75.683	92.837	-11.461	1.00	100.00	D
ATOM	5142	CB	ASP	D	203	76.079	91.426	-11.006	1.00	100.00	D
ATOM	5143	CG	ASP	D	203	77.131	90.790	-11.899	1.00	100.00	D
ATOM	5144	OD1	ASP	D	203	77.436	89.593	-11.693	1.00	100.00	D
ATOM	5145	OD2	ASP	D	203	77.650	91.483	-12.802	1.00	100.00	D
ATOM	5146	C	ASP	D	203	74.457	93.281	-10.667	1.00	100.00	D
ATOM	5147	O	ASP	D	203	74.540	94.312	-9.964	1.00	100.00	D
ATOM	5148	OXT	ASP	D	203	73.427	92.581	-10.755	1.00	100.00	D
ATOM	5149	C1	NAG	A	651	63.850	94.832	26.593	1.00	68.55	A
ATOM	5150	C2	NAG	A	651	63.632	94.709	28.104	1.00	68.55	A
ATOM	5151	N2	NAG	A	651	63.712	96.022	28.706	1.00	68.55	A
ATOM	5152	C7	NAG	A	651	62.733	96.458	29.489	1.00	68.55	A
ATOM	5153	O7	NAG	A	651	62.767	96.333	30.707	1.00	68.55	A
ATOM	5154	C8	NAG	A	651	61.541	97.145	28.833	1.00	68.55	A
ATOM	5155	C3	NAG	A	651	64.668	93.777	28.731	1.00	68.55	A
ATOM	5156	O3	NAG	A	651	64.408	93.631	30.120	1.00	68.55	A
ATOM	5157	C4	NAG	A	651	64.589	92.423	28.037	1.00	68.55	A
ATOM	5158	O4	NAG	A	651	65.540	91.503	28.618	1.00	68.55	A
ATOM	5159	C5	NAG	A	651	64.884	92.637	26.552	1.00	68.55	A
ATOM	5160	O5	NAG	A	651	63.898	93.531	25.975	1.00	68.55	A

FIGURE 2 Continued

ATOM	5161	C6	NAG	A	651	64.834	91.342	25.754	1.00	68.55	A
ATOM	5162	O6	NAG	A	651	63.504	90.789	25.810	1.00	68.55	A
ATOM	5163	C1	NAG	A	652	65.055	90.264	29.021	1.00	91.39	A
ATOM	5164	C2	NAG	A	652	66.236	89.366	29.427	1.00	91.39	A
ATOM	5165	N2	NAG	A	652	67.021	89.025	28.258	1.00	91.39	A
ATOM	5166	C7	NAG	A	652	67.846	89.914	27.717	1.00	91.39	A
ATOM	5167	O7	NAG	A	652	67.681	90.373	26.589	1.00	91.39	A
ATOM	5168	C8	NAG	A	652	69.048	90.346	28.545	1.00	91.39	A
ATOM	5169	C3	NAG	A	652	65.763	88.069	30.091	1.00	91.39	A
ATOM	5170	O3	NAG	A	652	66.883	87.363	30.607	1.00	91.39	A
ATOM	5171	C4	NAG	A	652	64.773	88.370	31.218	1.00	91.39	A
ATOM	5172	O4	NAG	A	652	64.258	87.153	31.745	1.00	91.39	A
ATOM	5173	C5	NAG	A	652	63.635	89.227	30.656	1.00	91.39	A
ATOM	5174	O5	NAG	A	652	64.168	90.468	30.138	1.00	91.39	A
ATOM	5175	C6	NAG	A	652	62.563	89.576	31.681	1.00	91.39	A
ATOM	5176	O6	NAG	A	652	63.108	90.271	32.795	1.00	91.39	A
ATOM	5177	C1	NAG	B	651	38.808	84.496	68.218	1.00	100.00	B
ATOM	5178	C2	NAG	B	651	38.502	84.541	66.698	1.00	100.00	B
ATOM	5179	N2	NAG	B	651	37.072	84.723	66.499	1.00	100.00	B
ATOM	5180	C7	NAG	B	651	36.568	84.920	65.283	1.00	100.00	B
ATOM	5181	O7	NAG	B	651	36.554	86.022	64.734	1.00	100.00	B
ATOM	5182	C8	NAG	B	651	35.979	83.713	64.570	1.00	100.00	B
ATOM	5183	C3	NAG	B	651	38.962	83.241	66.008	1.00	100.00	B
ATOM	5184	O3	NAG	B	651	38.856	83.380	64.598	1.00	100.00	B
ATOM	5185	C4	NAG	B	651	40.410	82.911	66.382	1.00	100.00	B
ATOM	5186	O4	NAG	B	651	40.783	81.657	65.828	1.00	100.00	B
ATOM	5187	C5	NAG	B	651	40.537	82.866	67.906	1.00	100.00	B
ATOM	5188	O5	NAG	B	651	40.186	84.151	68.459	1.00	100.00	B
ATOM	5189	C6	NAG	B	651	41.941	82.534	68.377	1.00	100.00	B
ATOM	5190	O6	NAG	B	651	42.198	81.140	68.280	1.00	100.00	B
ATOM	5191	C1	NAG	C	651	63.417	128.288	49.924	1.00	68.42	C
ATOM	5192	C2	NAG	C	651	64.708	129.119	49.891	1.00	68.42	C
ATOM	5193	N2	NAG	C	651	65.331	129.025	48.584	1.00	68.42	C
ATOM	5194	C7	NAG	C	651	65.531	130.125	47.864	1.00	68.42	C
ATOM	5195	O7	NAG	C	651	64.832	130.432	46.896	1.00	68.42	C
ATOM	5196	C8	NAG	C	651	66.688	131.026	48.280	1.00	68.42	C
ATOM	5197	C3	NAG	C	651	65.698	128.660	50.957	1.00	68.42	C
ATOM	5198	O3	NAG	C	651	66.807	129.548	50.985	1.00	68.42	C
ATOM	5199	C4	NAG	C	651	65.026	128.643	52.324	1.00	68.42	C
ATOM	5200	O4	NAG	C	651	65.942	128.124	53.313	1.00	68.42	C
ATOM	5201	C5	NAG	C	651	63.754	127.784	52.275	1.00	68.42	C
ATOM	5202	O5	NAG	C	651	62.859	128.275	51.250	1.00	68.42	C
ATOM	5203	C6	NAG	C	651	62.989	127.882	53.582	1.00	68.42	C
ATOM	5204	O6	NAG	C	651	62.608	129.258	53.793	1.00	68.42	C
ATOM	5205	C1	NAG	C	652	66.171	128.931	54.421	1.00	100.00	C
ATOM	5206	C2	NAG	C	652	66.861	128.115	55.522	1.00	100.00	C
ATOM	5207	N2	NAG	C	652	66.001	127.025	55.952	1.00	100.00	C
ATOM	5208	C7	NAG	C	652	64.979	127.252	56.776	1.00	100.00	C
ATOM	5209	O7	NAG	C	652	63.857	127.557	56.375	1.00	100.00	C
ATOM	5210	C8	NAG	C	652	65.241	127.124	58.273	1.00	100.00	C
ATOM	5211	C3	NAG	C	652	67.208	129.029	56.708	1.00	100.00	C
ATOM	5212	O3	NAG	C	652	67.940	128.302	57.686	1.00	100.00	C
ATOM	5213	C4	NAG	C	652	68.033	130.221	56.226	1.00	100.00	C
ATOM	5214	O4	NAG	C	652	68.262	131.117	57.305	1.00	100.00	C
ATOM	5215	C5	NAG	C	652	67.294	130.946	55.098	1.00	100.00	C

FIGURE 2 Continued

ATOM	5216	O5	NAG	C	652	67.011	130.026	54.016	1.00	100.00	C
ATOM	5217	C6	NAG	C	652	68.116	132.089	54.523	1.00	100.00	C
ATOM	5218	O6	NAG	C	652	67.664	132.452	53.228	1.00	100.00	C
ATOM	5219	C1	NAG	D	651	103.058	89.882	-9.969	1.00	74.98	D
ATOM	5220	C2	NAG	D	651	104.475	90.371	-10.345	1.00	74.98	D
ATOM	5221	N2	NAG	D	651	105.467	89.307	-10.332	1.00	74.98	D
ATOM	5222	C7	NAG	D	651	105.744	88.620	-9.224	1.00	74.98	D
ATOM	5223	O7	NAG	D	651	105.839	89.134	-8.096	1.00	74.98	D
ATOM	5224	C8	NAG	D	651	105.958	87.122	-9.400	1.00	74.98	D
ATOM	5225	C3	NAG	D	651	104.892	91.520	-9.434	1.00	74.98	D
ATOM	5226	O3	NAG	D	651	106.198	91.964	-9.777	1.00	74.98	D
ATOM	5227	C4	NAG	D	651	103.883	92.641	-9.633	1.00	74.98	D
ATOM	5228	O4	NAG	D	651	104.247	93.792	-8.844	1.00	74.98	D
ATOM	5229	C5	NAG	D	651	102.478	92.135	-9.255	1.00	74.98	D
ATOM	5230	O5	NAG	D	651	102.119	90.979	-10.064	1.00	74.98	D
ATOM	5231	C6	NAG	D	651	101.402	93.189	-9.485	1.00	74.98	D
ATOM	5232	O6	NAG	D	651	101.461	93.661	-10.848	1.00	74.98	D
ATOM	5233	C1	NAG	D	652	104.420	94.982	-9.546	1.00	98.85	D
ATOM	5234	C2	NAG	D	652	104.427	96.163	-8.568	1.00	98.85	D
ATOM	5235	N2	NAG	D	652	103.145	96.270	-7.902	1.00	98.85	D
ATOM	5236	C7	NAG	D	652	102.875	95.490	-6.862	1.00	98.85	D
ATOM	5237	O7	NAG	D	652	103.723	95.171	-6.025	1.00	98.85	D
ATOM	5238	C8	NAG	D	652	101.452	94.977	-6.736	1.00	98.85	D
ATOM	5239	C3	NAG	D	652	104.737	97.466	-9.310	1.00	98.85	D
ATOM	5240	O3	NAG	D	652	104.833	98.534	-8.381	1.00	98.85	D
ATOM	5241	C4	NAG	D	652	106.052	97.324	-10.071	1.00	98.85	D
ATOM	5242	O4	NAG	D	652	106.312	98.509	-10.814	1.00	98.85	D
ATOM	5243	C5	NAG	D	652	105.953	96.118	-11.013	1.00	98.85	D
ATOM	5244	O5	NAG	D	652	105.674	94.916	-10.251	1.00	98.85	D
ATOM	5245	C6	NAG	D	652	107.225	95.871	-11.810	1.00	98.85	D
ATOM	5246	O6	NAG	D	652	108.386	96.125	-11.032	1.00	98.85	D
ATOM	5247	C1	FUC	A	653	63.367	89.618	25.052	1.00	70.32	A
ATOM	5248	C2	FUC	A	653	62.115	88.863	25.509	1.00	70.32	A
ATOM	5249	O2	FUC	A	653	62.157	88.688	26.918	1.00	70.32	A
ATOM	5250	C3	FUC	A	653	60.856	89.646	25.132	1.00	70.32	A
ATOM	5251	O3	FUC	A	653	59.707	88.879	25.450	1.00	70.32	A
ATOM	5252	C4	FUC	A	653	60.850	89.986	23.639	1.00	70.32	A
ATOM	5253	O4	FUC	A	653	60.667	88.804	22.877	1.00	70.32	A
ATOM	5254	C5	FUC	A	653	62.166	90.672	23.234	1.00	70.32	A
ATOM	5255	O5	FUC	A	653	63.300	89.875	23.649	1.00	70.32	A
ATOM	5256	C6	FUC	A	653	62.282	90.868	21.734	1.00	70.32	A
ATOM	5257	C1	FUC	C	653	62.005	129.498	55.033	1.00	71.31	C
ATOM	5258	C2	FUC	C	653	62.082	131.004	55.367	1.00	71.31	C
ATOM	5259	O2	FUC	C	653	63.420	131.466	55.253	1.00	71.31	C
ATOM	5260	C3	FUC	C	653	61.176	131.788	54.416	1.00	71.31	C
ATOM	5261	O3	FUC	C	653	61.234	133.176	54.705	1.00	71.31	C
ATOM	5262	C4	FUC	C	653	59.751	131.272	54.572	1.00	71.31	C
ATOM	5263	O4	FUC	C	653	59.330	131.451	55.920	1.00	71.31	C
ATOM	5264	C5	FUC	C	653	59.734	129.781	54.214	1.00	71.31	C
ATOM	5265	O5	FUC	C	653	60.646	129.049	55.072	1.00	71.31	C
ATOM	5266	C6	FUC	C	653	58.364	129.152	54.372	1.00	71.31	C
ATOM	5267	C1	FUC	D	653	100.642	94.777	-11.078	1.00	71.23	D
ATOM	5268	C2	FUC	D	653	101.026	95.446	-12.409	1.00	71.23	D
ATOM	5269	O2	FUC	D	653	102.420	95.729	-12.432	1.00	71.23	D
ATOM	5270	C3	FUC	D	653	100.660	94.525	-13.578	1.00	71.23	D

FIGURE 2 Continued

ATOM	5271	O3	FUC	D	653	100.963	95.158	-14.814	1.00	71.23	D
ATOM	5272	C4	FUC	D	653	99.170	94.171	-13.518	1.00	71.23	D
ATOM	5273	O4	FUC	D	653	98.381	95.335	-13.727	1.00	71.23	D
ATOM	5274	C5	FUC	D	653	98.836	93.557	-12.154	1.00	71.23	D
ATOM	5275	O5	FUC	D	653	99.251	94.443	-11.083	1.00	71.23	D
ATOM	5276	C6	FUC	D	653	97.349	93.319	-11.988	1.00	71.23	D
ATOM	5277	S	SO4	S	290	87.269	114.471	20.201	1.00	56.53	S
ATOM	5278	O1	SO4	S	290	87.763	114.116	18.855	1.00	56.53	S
ATOM	5279	O2	SO4	S	290	85.981	113.803	20.472	1.00	56.53	S
ATOM	5280	O3	SO4	S	290	87.066	115.930	20.260	1.00	56.53	S
ATOM	5281	O4	SO4	S	290	88.255	114.036	21.209	1.00	56.53	S
ATOM	5282	S	SO4	S	291	65.177	99.186	80.678	1.00	100.00	S
ATOM	5283	O1	SO4	S	291	63.867	99.855	80.809	1.00	100.00	S
ATOM	5284	O2	SO4	S	291	64.972	97.810	80.181	1.00	100.00	S
ATOM	5285	O3	SO4	S	291	65.834	99.154	81.999	1.00	100.00	S
ATOM	5286	O4	SO4	S	291	66.036	99.927	79.733	1.00	100.00	S
ATOM	5287	S	SO4	S	292	64.193	99.447	37.657	1.00	60.46	S
ATOM	5288	O1	SO4	S	292	65.362	98.575	37.866	1.00	60.46	S
ATOM	5289	O2	SO4	S	292	63.121	99.042	38.580	1.00	60.46	S
ATOM	5290	O3	SO4	S	292	63.707	99.332	36.270	1.00	60.46	S
ATOM	5291	O4	SO4	S	292	64.581	100.841	37.921	1.00	60.46	S
ATOM	5292	S	SO4	S	293	98.600	73.817	16.564	1.00	49.60	S
ATOM	5293	O1	SO4	S	293	99.493	74.314	17.627	1.00	49.60	S
ATOM	5294	O2	SO4	S	293	97.218	74.226	16.862	1.00	49.60	S
ATOM	5295	O3	SO4	S	293	98.678	72.341	16.514	1.00	49.60	S
ATOM	5296	O4	SO4	S	293	99.000	74.391	15.270	1.00	49.60	S
ATOM	5297	S	SO4	S	294	80.532	120.977	15.256	1.00	99.04	S
ATOM	5298	O1	SO4	S	294	81.699	121.011	16.163	1.00	99.04	S
ATOM	5299	O2	SO4	S	294	80.210	122.351	14.830	1.00	99.04	S
ATOM	5300	O3	SO4	S	294	79.358	120.395	15.944	1.00	99.04	S
ATOM	5301	O4	SO4	S	294	80.877	120.171	14.069	1.00	99.04	S
ATOM	5302	S	SO4	S	295	58.950	102.740	88.312	1.00	100.00	S
ATOM	5303	O1	SO4	S	295	59.842	102.968	87.152	1.00	100.00	S
ATOM	5304	O2	SO4	S	295	59.774	102.431	89.502	1.00	100.00	S
ATOM	5305	O3	SO4	S	295	58.041	101.603	88.032	1.00	100.00	S
ATOM	5306	O4	SO4	S	295	58.149	103.959	88.562	1.00	100.00	S
ATOM	5307	S	SO4	S	296	57.564	103.837	30.030	1.00	100.00	S
ATOM	5308	O1	SO4	S	296	58.893	103.618	29.431	1.00	100.00	S
ATOM	5309	O2	SO4	S	296	56.598	104.166	28.960	1.00	100.00	S
ATOM	5310	O3	SO4	S	296	57.633	104.962	30.989	1.00	100.00	S
ATOM	5311	O4	SO4	S	296	57.134	102.604	30.726	1.00	100.00	S
ATOM	5312	S	SO4	S	297	96.037	65.451	9.537	1.00	90.21	S
ATOM	5313	O1	SO4	S	297	97.355	64.786	9.509	1.00	90.21	S
ATOM	5314	O2	SO4	S	297	96.063	66.627	8.645	1.00	90.21	S
ATOM	5315	O3	SO4	S	297	95.715	65.864	10.919	1.00	90.21	S
ATOM	5316	O4	SO4	S	297	95.007	64.512	9.057	1.00	90.21	S
ATOM	5317	OH2	WAT	W	1	98.243	72.793	8.778	1.00	40.14	W
ATOM	5318	OH2	WAT	W	2	100.723	99.069	1.343	1.00	43.74	W
ATOM	5319	OH2	WAT	W	3	82.241	105.217	19.713	1.00	28.74	W
ATOM	5320	OH2	WAT	W	4	75.884	89.321	17.720	1.00	28.05	W
ATOM	5321	OH2	WAT	W	5	93.183	80.024	16.428	1.00	24.14	W
ATOM	5322	OH2	WAT	W	6	77.336	105.675	24.395	1.00	32.73	W
ATOM	5323	OH2	WAT	W	7	69.995	85.178	19.215	1.00	45.10	W
ATOM	5324	OH2	WAT	W	8	72.713	111.831	18.813	1.00	28.44	W
ATOM	5325	OH2	WAT	W	9	70.462	97.602	28.514	1.00	38.75	W

FIGURE 2 Continued

ATOM	5326	OH2	WAT	W	10	81.728	86.681	-4.948	1.00	46.77	W
ATOM	5327	OH2	WAT	W	11	46.060	107.671	59.577	1.00	64.17	W
ATOM	5328	OH2	WAT	W	12	84.139	88.047	23.458	1.00	64.93	W
ATOM	5329	OH2	WAT	W	13	60.994	118.607	32.498	1.00	45.07	W
ATOM	5330	OH2	WAT	W	14	65.151	112.020	43.183	1.00	38.22	W
ATOM	5331	OH2	WAT	W	15	101.436	76.882	21.919	1.00	43.89	W
ATOM	5332	OH2	WAT	W	16	70.692	82.671	2.951	1.00	39.40	W
ATOM	5333	OH2	WAT	W	17	77.880	90.837	6.039	1.00	45.30	W
ATOM	5334	OH2	WAT	W	18	53.388	120.527	54.360	1.00	32.92	W
ATOM	5335	OH2	WAT	W	19	88.455	87.041	22.408	1.00	48.72	W
ATOM	5336	OH2	WAT	W	20	62.755	109.918	29.364	1.00	45.86	W
ATOM	5337	OH2	WAT	W	21	101.357	76.280	16.232	1.00	31.46	W
ATOM	5338	OH2	WAT	W	22	80.811	81.779	-1.444	1.00	45.90	W
ATOM	5339	OH2	WAT	W	23	54.512	121.498	52.129	1.00	43.52	W
ATOM	5340	OH2	WAT	W	24	95.558	95.007	-15.047	1.00	62.31	W
ATOM	5341	OH2	WAT	W	25	70.709	120.756	37.731	1.00	47.56	W
ATOM	5342	OH2	WAT	W	26	58.731	102.298	42.435	1.00	40.62	W
ATOM	5343	OH2	WAT	W	27	102.361	62.548	12.953	1.00	50.77	W
ATOM	5344	OH2	WAT	W	28	111.776	66.358	13.734	1.00	35.34	W
ATOM	5345	OH2	WAT	W	29	89.104	92.829	16.621	1.00	40.61	W
ATOM	5346	OH2	WAT	W	30	43.225	109.666	46.636	1.00	54.75	W
ATOM	5347	OH2	WAT	W	31	67.323	94.804	16.042	1.00	38.16	W
ATOM	5348	OH2	WAT	W	32	59.324	121.006	34.693	1.00	43.79	W
ATOM	5349	OH2	WAT	W	33	82.453	77.000	9.480	1.00	54.51	W
ATOM	5350	OH2	WAT	W	34	95.982	100.629	12.897	1.00	47.38	W
ATOM	5351	OH2	WAT	W	35	54.160	113.078	74.080	1.00	63.51	W
ATOM	5352	OH2	WAT	W	36	68.861	92.681	14.691	1.00	36.90	W
ATOM	5353	OH2	WAT	W	37	96.636	81.840	10.110	1.00	25.09	W
ATOM	5354	OH2	WAT	W	38	108.927	91.327	8.447	1.00	44.64	W
ATOM	5355	OH2	WAT	W	39	80.800	92.167	3.134	1.00	51.75	W
ATOM	5356	OH2	WAT	W	40	91.129	102.744	28.200	1.00	37.60	W
ATOM	5357	OH2	WAT	W	41	79.061	91.827	-0.696	1.00	39.58	W
ATOM	5358	OH2	WAT	W	42	55.591	110.935	65.257	1.00	61.81	W
ATOM	5359	OH2	WAT	W	43	88.416	107.977	9.153	1.00	40.78	W
ATOM	5360	OH2	WAT	W	44	49.615	85.837	59.269	1.00	58.95	W
ATOM	5361	OH2	WAT	W	45	88.447	107.397	16.191	1.00	33.70	W
ATOM	5362	OH2	WAT	W	46	62.234	106.156	45.413	1.00	36.64	W
ATOM	5363	OH2	WAT	W	47	76.054	93.988	16.647	1.00	28.00	W
ATOM	5364	OH2	WAT	W	48	61.293	106.411	36.257	1.00	38.13	W
ATOM	5365	OH2	WAT	W	49	84.935	101.229	8.292	1.00	37.11	W
ATOM	5366	OH2	WAT	W	50	73.442	104.943	26.714	1.00	37.40	W
ATOM	5367	OH2	WAT	W	51	62.168	109.685	18.951	1.00	58.71	W
ATOM	5368	OH2	WAT	W	52	86.134	99.036	9.586	1.00	39.95	W
ATOM	5369	OH2	WAT	W	53	53.297	114.656	43.291	1.00	34.32	W
ATOM	5370	OH2	WAT	W	54	91.965	91.169	2.028	1.00	28.84	W
ATOM	5371	OH2	WAT	W	55	68.554	106.631	38.047	1.00	29.96	W
ATOM	5372	OH2	WAT	W	56	42.275	117.236	51.563	1.00	55.68	W
ATOM	5373	OH2	WAT	W	57	78.710	113.956	1.464	1.00	52.50	W
ATOM	5374	OH2	WAT	W	58	67.208	114.504	23.283	1.00	43.10	W
ATOM	5375	OH2	WAT	W	59	82.994	99.681	31.729	1.00	48.60	W
ATOM	5376	OH2	WAT	W	60	65.200	109.879	24.059	1.00	60.10	W
ATOM	5377	OH2	WAT	W	61	97.040	73.278	2.059	1.00	45.25	W
ATOM	5378	OH2	WAT	W	62	93.225	99.035	-5.528	1.00	49.05	W
ATOM	5379	OH2	WAT	W	63	71.875	100.135	3.573	1.00	46.15	W
ATOM	5380	OH2	WAT	W	64	62.928	104.236	22.446	1.00	52.64	W

FIGURE 2 Continued

ATOM	5381	OH2	WAT	W	65	44.217	112.617	48.777	1.00	48.56	W
ATOM	5382	OH2	WAT	W	66	93.228	67.203	7.652	1.00	41.59	W
ATOM	5383	OH2	WAT	W	67	77.650	103.578	32.499	1.00	40.82	W
ATOM	5384	OH2	WAT	W	68	91.335	94.124	22.779	1.00	59.93	W
ATOM	5385	OH2	WAT	W	69	48.083	109.798	59.363	1.00	57.31	W
ATOM	5386	OH2	WAT	W	70	58.427	112.971	36.462	1.00	34.49	W
ATOM	5387	OH2	WAT	W	71	103.742	87.373	18.534	1.00	41.96	W
ATOM	5388	OH2	WAT	W	72	83.955	83.619	7.649	1.00	36.86	W
ATOM	5389	OH2	WAT	W	73	105.879	85.929	18.515	1.00	58.34	W
ATOM	5390	OH2	WAT	W	74	73.385	114.693	44.497	1.00	50.73	W
ATOM	5391	OH2	WAT	W	75	90.898	81.250	21.569	1.00	53.51	W
ATOM	5392	OH2	WAT	W	76	93.172	77.536	12.194	1.00	34.23	W
ATOM	5393	OH2	WAT	W	77	71.336	105.163	13.459	1.00	39.65	W
ATOM	5394	OH2	WAT	W	78	94.872	75.387	12.718	1.00	27.22	W
ATOM	5395	OH2	WAT	W	79	79.491	113.953	19.501	1.00	41.09	W
ATOM	5396	OH2	WAT	W	80	73.163	112.199	16.131	1.00	31.19	W
ATOM	5397	OH2	WAT	W	81	81.906	111.926	26.496	1.00	33.98	W
ATOM	5398	OH2	WAT	W	82	70.470	89.549	20.238	1.00	40.29	W
ATOM	5399	OH2	WAT	W	83	93.047	104.689	7.488	1.00	48.34	W
ATOM	5400	OH2	WAT	W	84	104.406	76.662	11.032	1.00	29.83	W
ATOM	5401	OH2	WAT	W	85	84.174	109.256	15.552	1.00	28.81	W
ATOM	5402	OH2	WAT	W	86	90.192	90.721	-5.640	1.00	54.35	W
ATOM	5403	OH2	WAT	W	87	85.476	86.441	12.601	1.00	30.66	W
ATOM	5404	OH2	WAT	W	88	67.390	95.645	3.293	1.00	44.86	W
ATOM	5405	OH2	WAT	W	89	102.338	75.732	13.813	1.00	41.56	W
ATOM	5406	OH2	WAT	W	90	92.271	95.700	0.716	1.00	36.78	W
ATOM	5407	OH2	WAT	W	91	82.997	77.296	6.765	1.00	38.94	W
ATOM	5408	OH2	WAT	W	92	67.517	83.159	2.651	1.00	50.39	W
ATOM	5409	OH2	WAT	W	93	101.590	81.432	5.335	1.00	32.29	W
ATOM	5410	OH2	WAT	W	94	61.174	108.116	16.606	1.00	41.44	W
ATOM	5411	OH2	WAT	W	95	64.720	114.974	12.791	1.00	44.59	W
ATOM	5412	OH2	WAT	W	96	78.195	117.163	28.367	1.00	40.57	W
ATOM	5413	OH2	WAT	W	97	57.717	114.079	55.035	1.00	36.92	W
ATOM	5414	OH2	WAT	W	98	67.044	100.744	39.547	1.00	51.71	W
ATOM	5415	OH2	WAT	W	99	92.153	88.819	-6.463	1.00	42.00	W
ATOM	5416	OH2	WAT	W	100	83.503	119.049	18.338	1.00	39.68	W
ATOM	5417	OH2	WAT	W	101	84.247	111.886	16.564	1.00	34.46	W
ATOM	5418	OH2	WAT	W	102	84.120	114.466	15.058	1.00	46.29	W
ATOM	5419	OH2	WAT	W	103	78.739	92.710	1.767	1.00	53.05	W
ATOM	5420	OH2	WAT	W	104	75.383	119.594	22.530	1.00	45.72	W
ATOM	5421	OH2	WAT	W	105	97.340	99.403	8.650	1.00	59.09	W
ATOM	5422	OH2	WAT	W	106	60.487	98.834	45.196	1.00	48.04	W
ATOM	5423	OH2	WAT	W	107	81.895	97.296	33.308	1.00	53.41	W
ATOM	5424	OH2	WAT	W	108	61.463	106.999	18.809	1.00	46.26	W
ATOM	5425	OH2	WAT	W	109	103.807	87.900	14.867	1.00	42.52	W
ATOM	5426	OH2	WAT	W	110	61.631	121.926	36.087	1.00	57.28	W
ATOM	5427	OH2	WAT	W	111	80.906	98.367	7.256	1.00	39.55	W
ATOM	5428	OH2	WAT	W	112	84.738	112.744	24.379	1.00	37.45	W
ATOM	5429	OH2	WAT	W	113	97.371	95.058	17.386	1.00	45.28	W
ATOM	5430	OH2	WAT	W	114	85.143	89.014	11.475	1.00	46.64	W
ATOM	5431	OH2	WAT	W	115	91.391	78.713	-1.122	1.00	25.77	W
ATOM	5432	OH2	WAT	W	116	103.551	81.877	1.731	1.00	50.24	W
ATOM	5433	OH2	WAT	W	117	43.228	107.507	36.707	1.00	52.06	W
ATOM	5434	OH2	WAT	W	118	93.991	67.254	13.175	1.00	55.01	W
ATOM	5435	OH2	WAT	W	119	47.508	104.474	44.657	1.00	42.36	W

FIGURE 2 Continued

ATOM	5436	OH2	WAT	W	120	93.716	103.969	19.726	1.00	48.72	W
ATOM	5437	OH2	WAT	W	121	96.426	74.427	-6.268	1.00	40.69	W
ATOM	5438	OH2	WAT	W	122	92.951	102.931	2.648	1.00	49.76	W
ATOM	5439	OH2	WAT	W	123	52.043	107.168	67.763	1.00	55.50	W
ATOM	5440	OH2	WAT	W	124	94.885	68.428	15.049	1.00	52.06	W
ATOM	5441	OH2	WAT	W	125	94.068	106.686	14.846	1.00	51.39	W
ATOM	5442	OH2	WAT	W	126	69.295	109.470	32.249	1.00	40.55	W
ATOM	5443	OH2	WAT	W	127	50.780	105.242	50.558	1.00	54.72	W
ATOM	5444	OH2	WAT	W	128	76.875	87.787	26.823	1.00	29.07	W
ATOM	5445	OH2	WAT	W	129	83.439	85.902	7.118	1.00	30.78	W
ATOM	5446	OH2	WAT	W	130	93.888	72.716	13.851	1.00	44.58	W
ATOM	5447	OH2	WAT	W	131	70.603	103.872	36.649	1.00	49.76	W
ATOM	5448	OH2	WAT	W	132	95.627	71.658	15.900	1.00	47.50	W
ATOM	5449	OH2	WAT	W	133	90.727	109.854	24.313	1.00	37.36	W
ATOM	5450	OH2	WAT	W	134	66.795	109.939	62.274	1.00	60.58	W
ATOM	5451	OH2	WAT	W	135	74.204	77.679	2.581	1.00	60.35	W
ATOM	5452	OH2	WAT	W	136	82.625	107.558	4.030	1.00	40.37	W
ATOM	5453	OH2	WAT	W	137	72.941	97.648	39.459	1.00	48.32	W
ATOM	5454	OH2	WAT	W	138	60.515	81.451	72.811	1.00	60.18	W
ATOM	5455	OH2	WAT	W	139	83.361	104.042	35.263	1.00	49.95	W
ATOM	5456	OH2	WAT	W	140	111.952	86.558	10.762	1.00	48.42	W
ATOM	5457	OH2	WAT	W	141	77.317	110.318	45.555	1.00	59.12	W

END

FIGURE 3

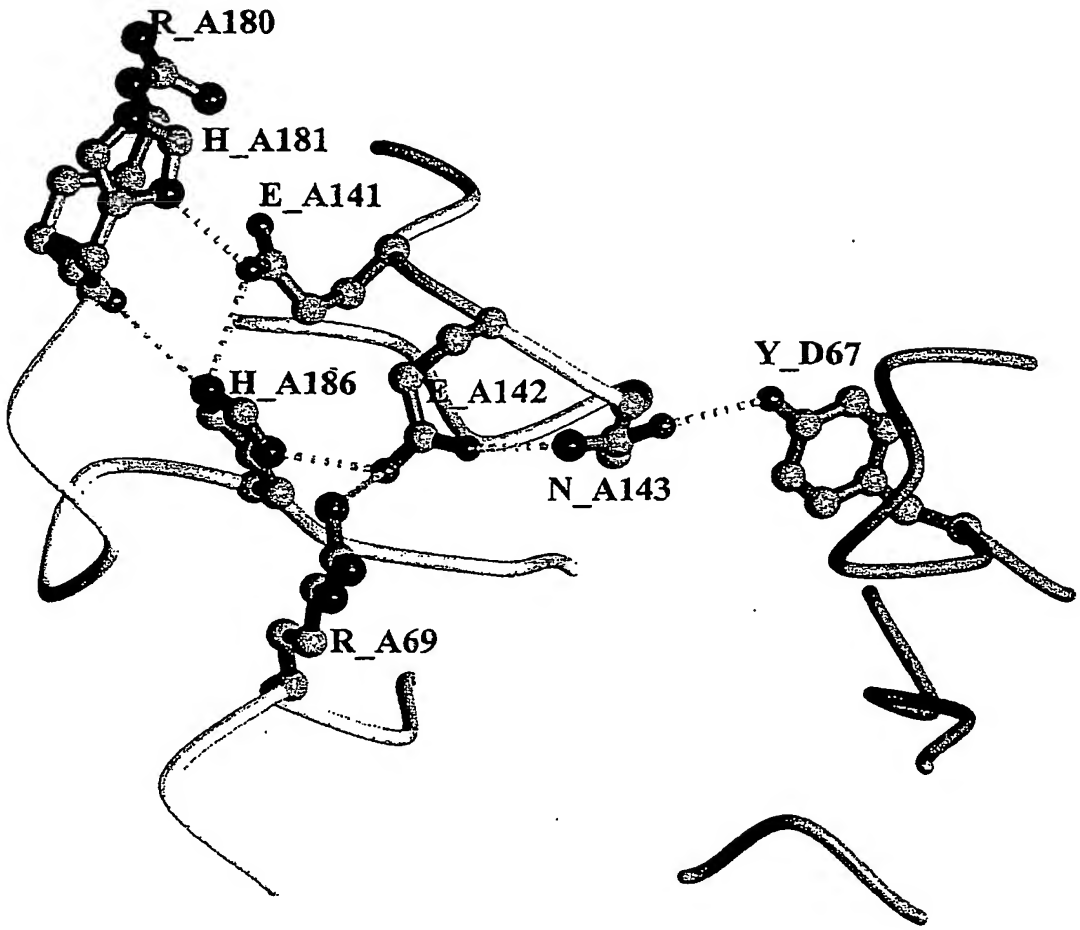
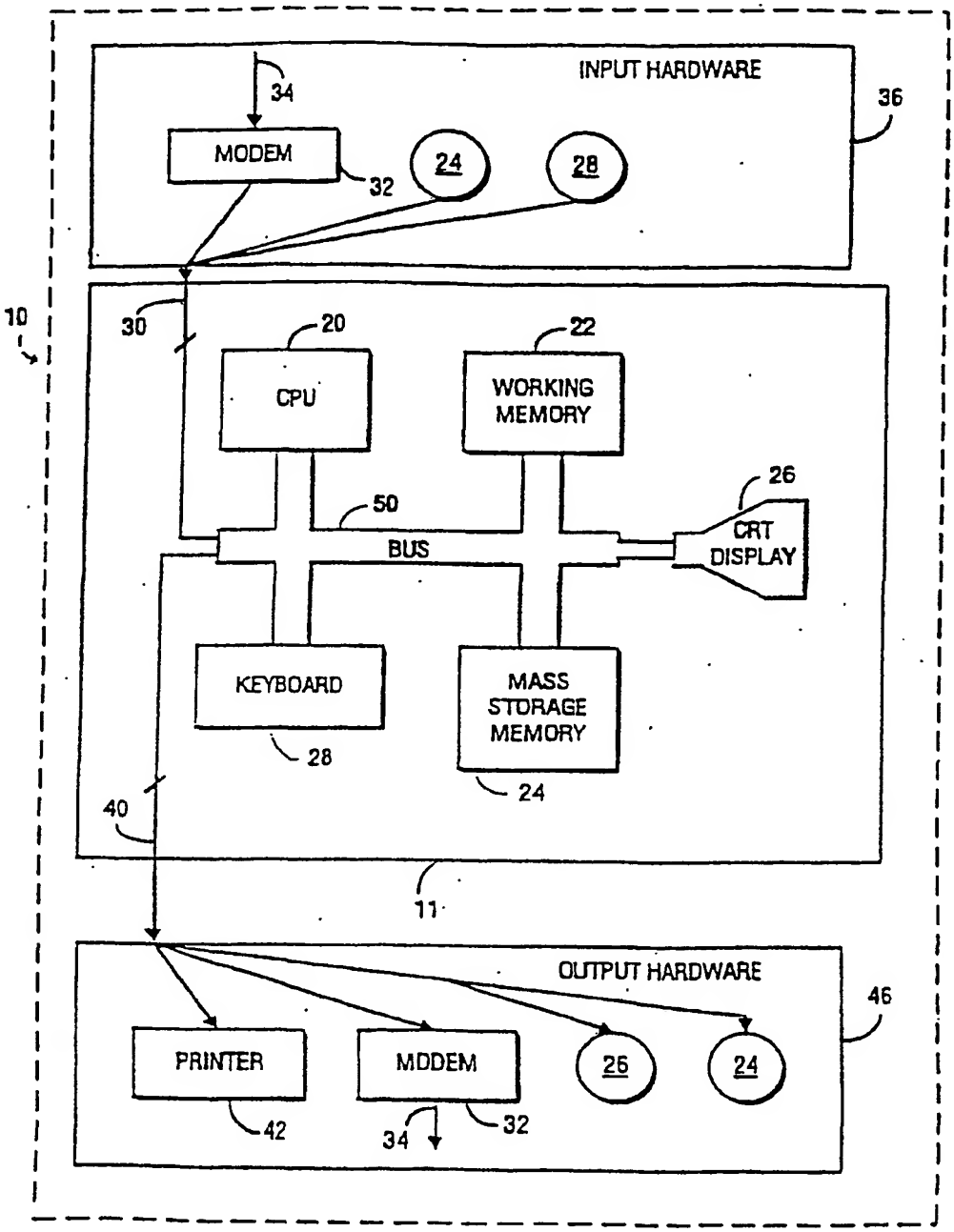


FIGURE 4


INPUT HARDWARE
34
36
MODEM
32
24
28
10
30
20
22
CPU
WORKING MEMORY
26
50
BUS
CRT DISPLAY
KEYBOARD
MASS STORAGE MEMORY
28
24
40
11
OUTPUT HARDWARE
46
PRINTER
MODEM
26
24
42
34
32

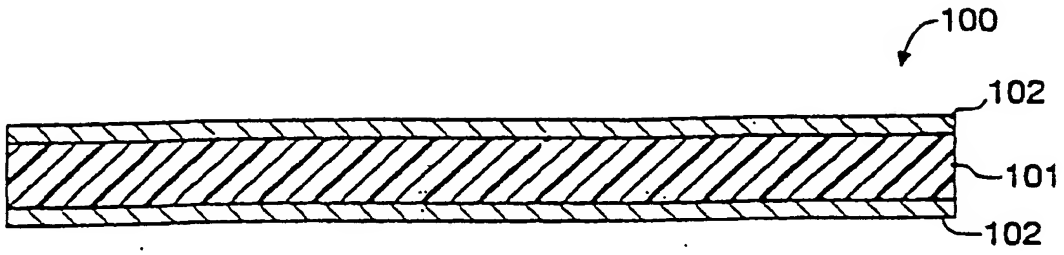


FIGURE 5A

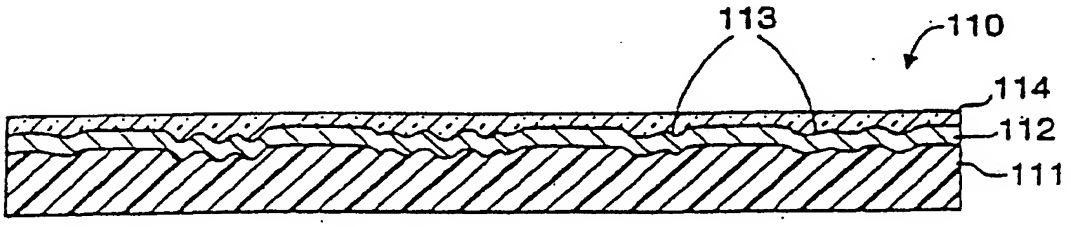


FIGURE 5B